

Efficient Particle-In-Cell algorithms for the modeling of advanced accelerators

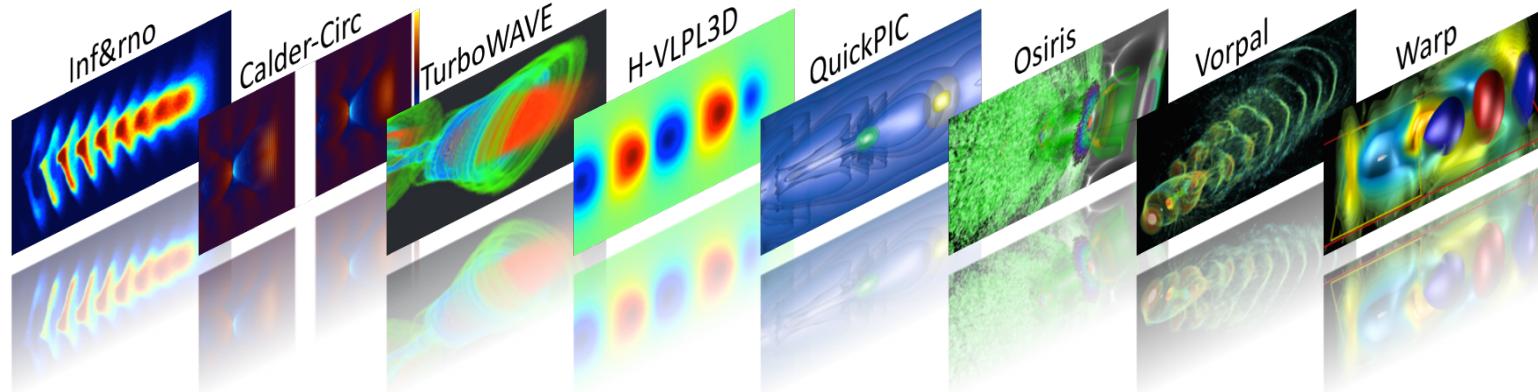
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with contributions from

C. Benedetti, D. Bruhwiler, E. Cormier-Michel, B. Cowan,

R. Fonseca, D. Gordon, A. Lifschitz, W. Mori



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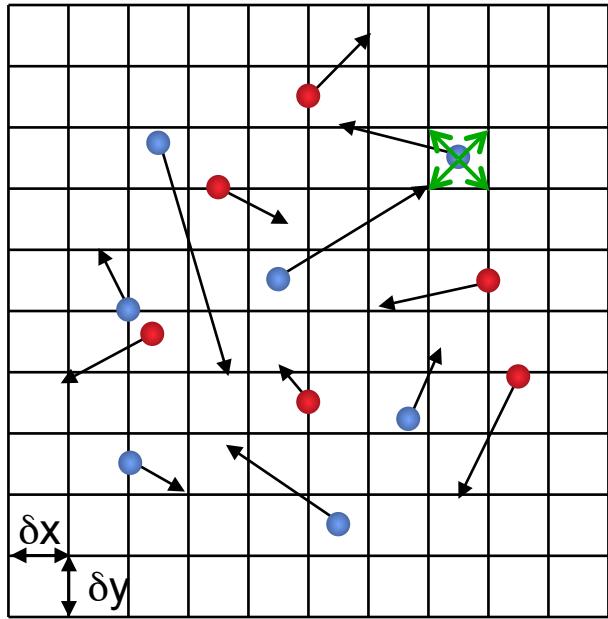
LAWRENCE BERKELEY NATIONAL LABORATORY



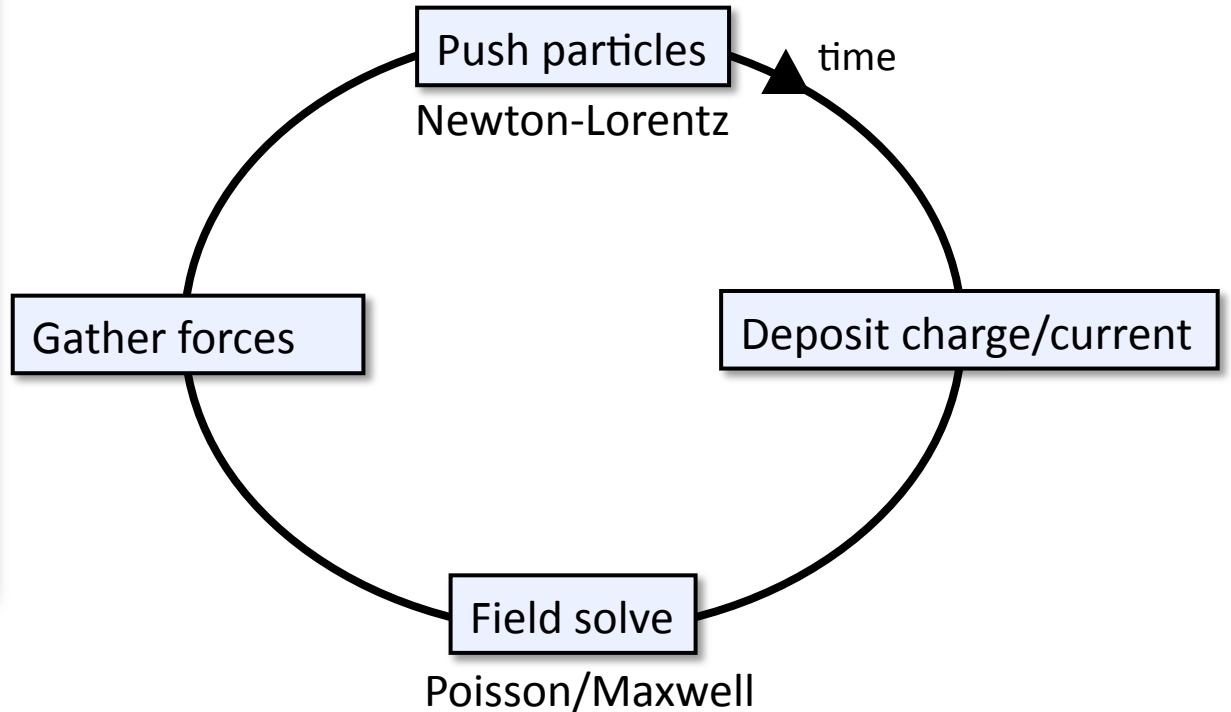
Outline

- Particle-In-Cell (PIC) method and challenges (focusing on laser plasma acceleration)
- Update on some new techniques & codes
 - improvements in speed, accuracy
 - mitigation of numerical instability
- Conclusion

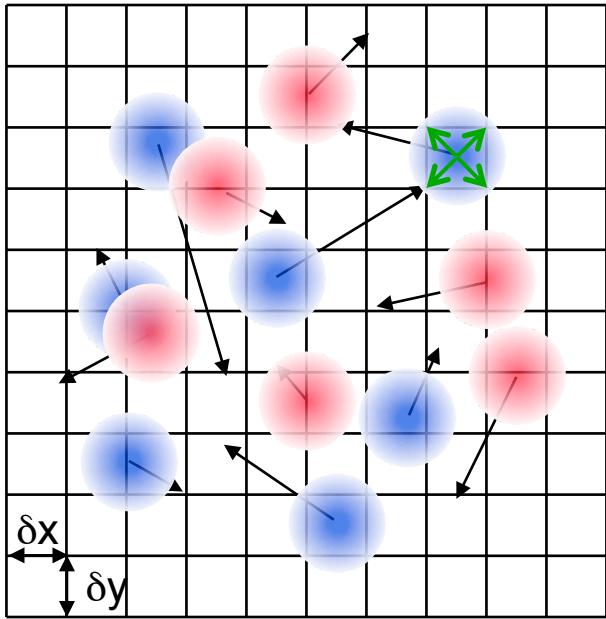
Particle-In-Cell workflow



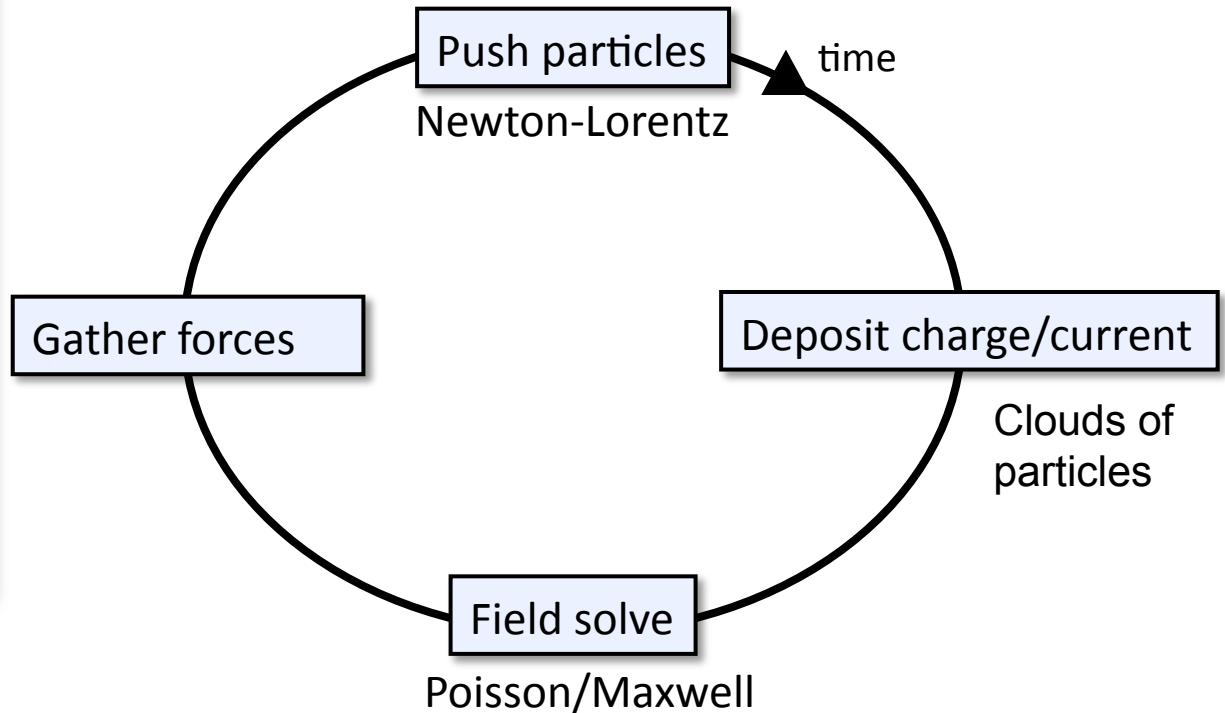
Plasma=collection of interacting charged particles



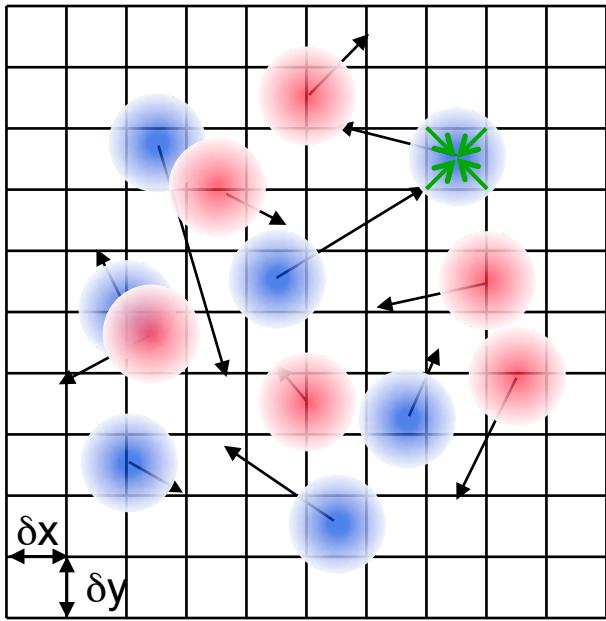
Particle-In-Cell workflow



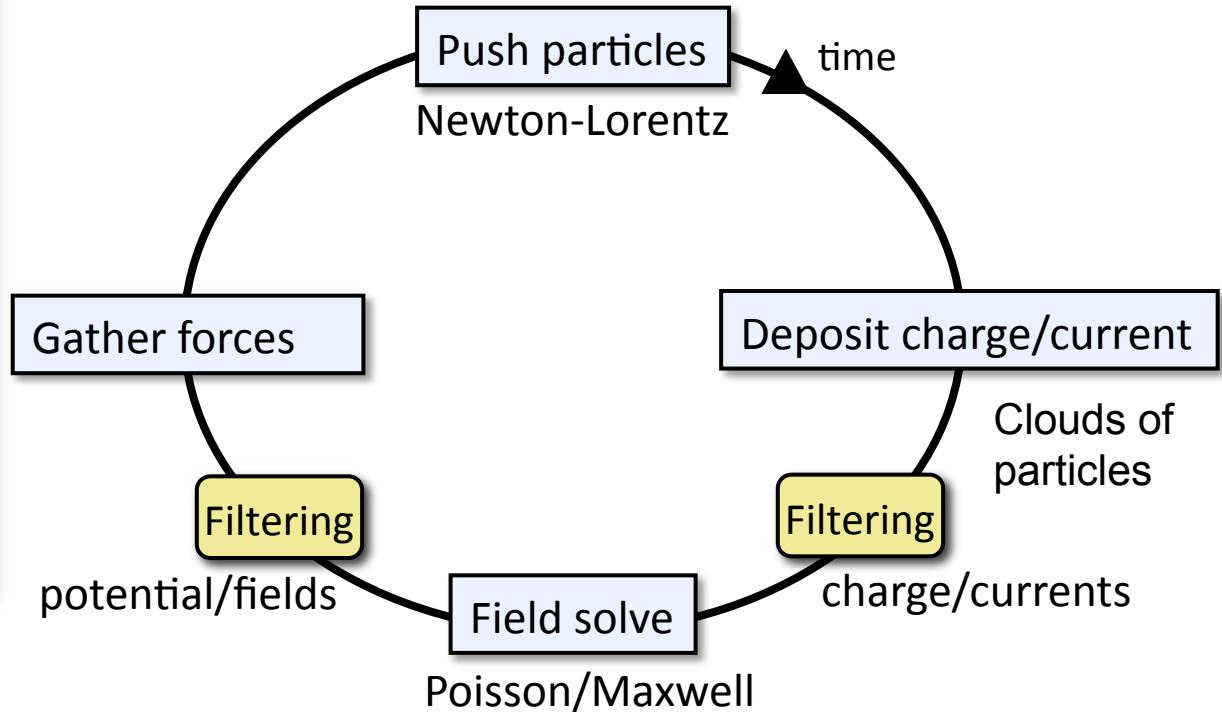
Plasma=collection of interacting charged particles



Particle-In-Cell workflow



Plasma=collection of interacting charged particles

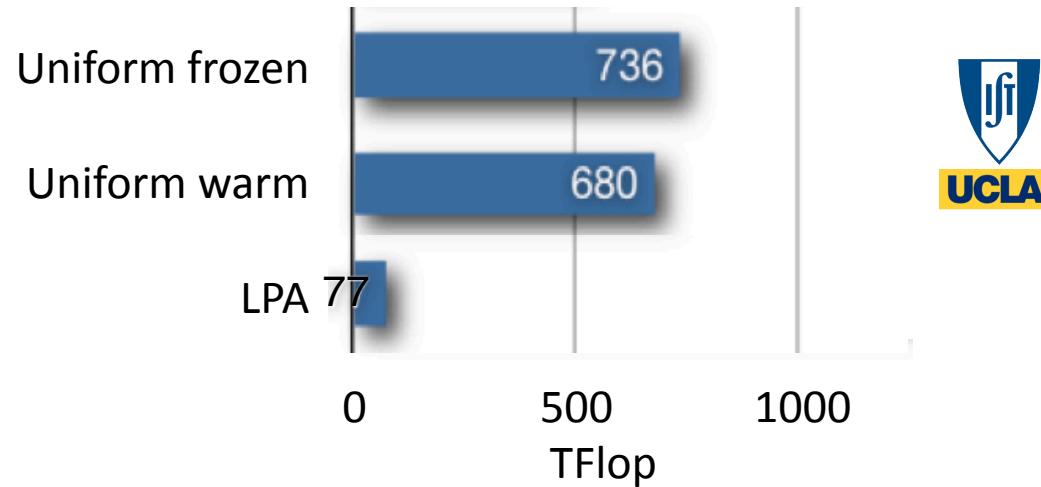


Time step is limited by stability limits:

- electron plasma frequency: $\delta t < 2/\omega_{pe}$
- electromagnetic: time for light to cross one cell $c \delta t < \delta x$

Uniform plasma PIC runs efficiently on largest supercomputers

- OSIRIS: OASCR full system tests on ORNL Jaguar supercomputer
 - up-to 740 Tflops (32% of peak) for uniform plasma test case
 - up-to 77 Tflops (3.3% of peak) for laser plasma acceleration (LPA) case



- See also talk from R. Fonseca (WG2)

not fast enough for “brute force” lab frame full PIC 10 GeV stage

→ need for better/faster algorithms and reduced models.

Laser plasma acceleration especially challenging

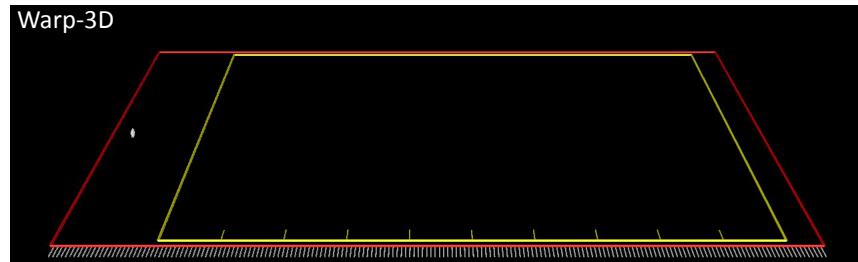
▪ Numerical limitations

- discretization errors (finite cell size, finite time step, staggering of quantities)
→ high resolution, small time steps and/or better algorithms
- sampling errors (noise)
→ many macroparticles and/or smoothing/filtering

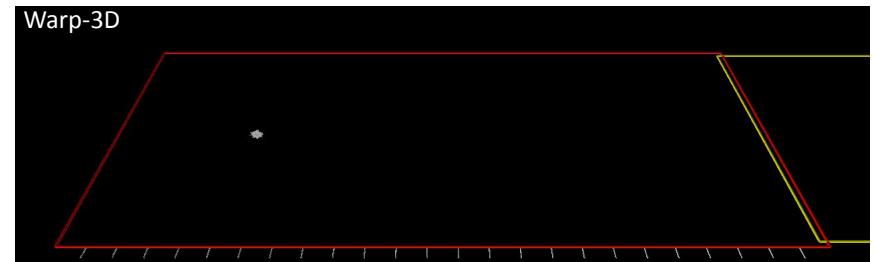
▪ Large space and time scale disparities

- **short** wavelength laser propagates into **long** plasma channel

Lab (full)



Lab (w/ moving window)



even with moving window, many time steps necessary for first principles simulations

(tens of millions of time steps for 10 GeV stage)

Dealing with large spatial/time scale disparities

Many techniques available:

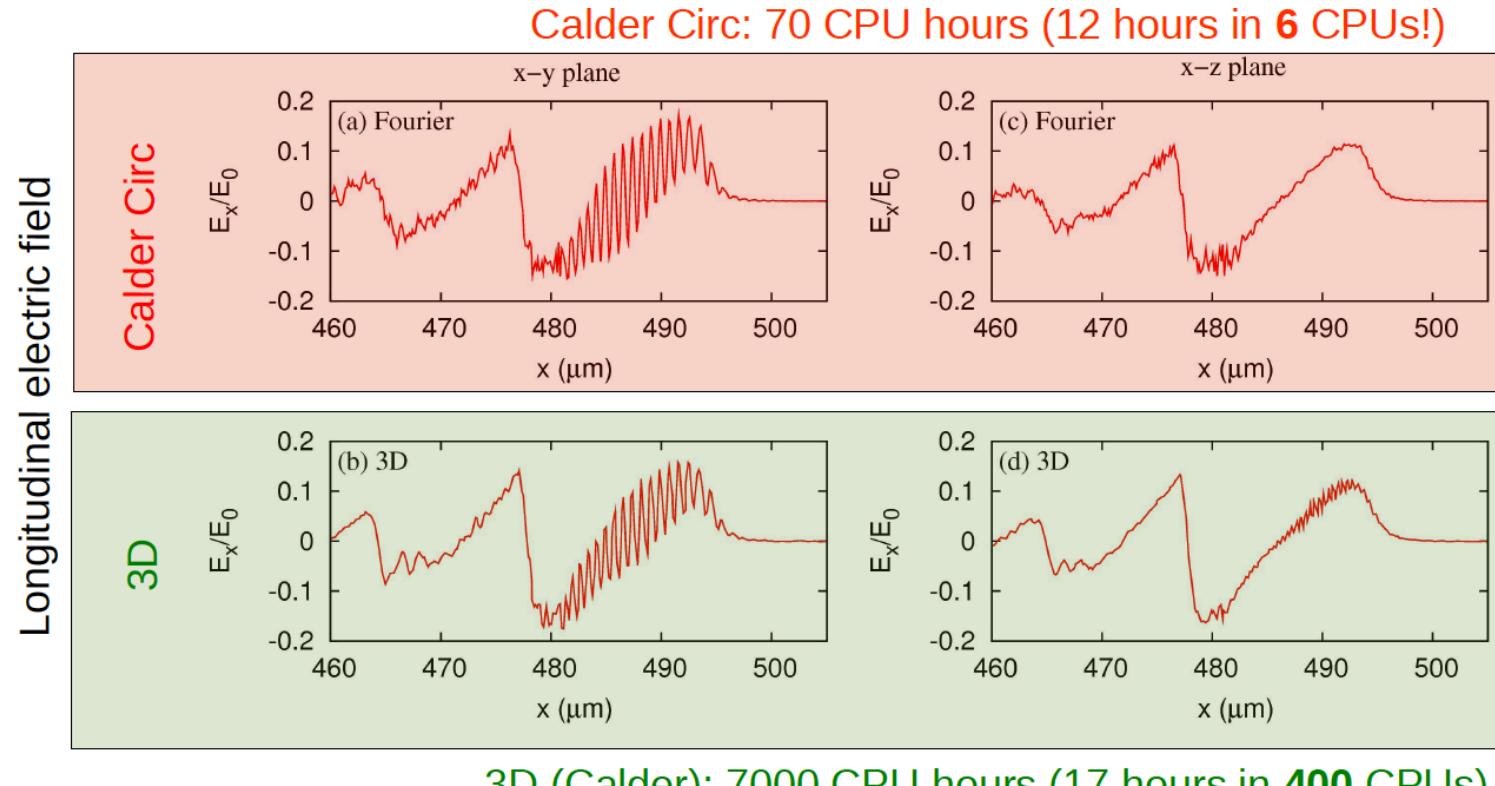
- downscaled parameters
 - e.g. LPA: 100 MeV/ 10^{19}cm^{-3} stage proxy for 10 GeV/ 10^{17}cm^{-3} stage
- reduced dimensionality: 1D, 2D, 2D-RZ, 2D-multimodes, fluid
- large time scale disparities
 - envelope/ponderomotive – averages over shortest time scale
 - quasistatic – separates slow macro- & fast micro-evolutions
 - Lorentz boosted frame – reduces scale disparities
- large spatial disparities
 - parallelization
 - moving window
 - mesh refinement

Update on various advances in following slides.

Reduced dimensionality

Calder-Circ*: PIC code based on θ -Fourier expansion

-- good agreement with 3D with cost close to 2D



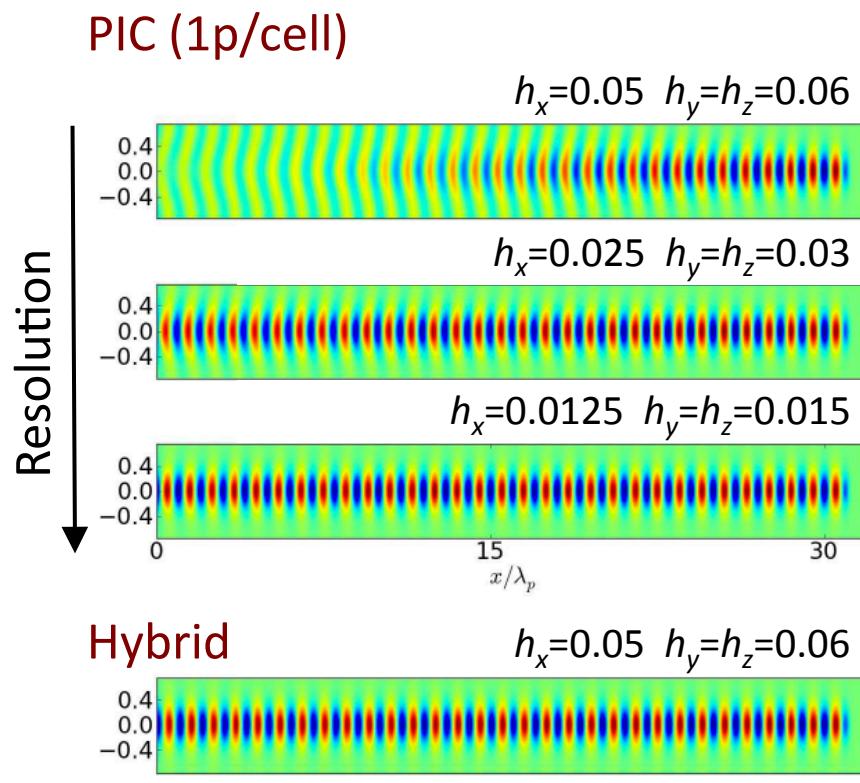
Fields are developed in azimuthal Fourier expansion

- mode $m=0 \rightarrow$ axially symmetric wakefield
 - mode $m=1 \rightarrow$ laser
 - 2 modes are enough to model the laser-plasma interaction in underdense plasmas
- $$E = \Re \left(\sum_{m=0}^M E^m(r, z) \exp(-im\theta) \right)$$

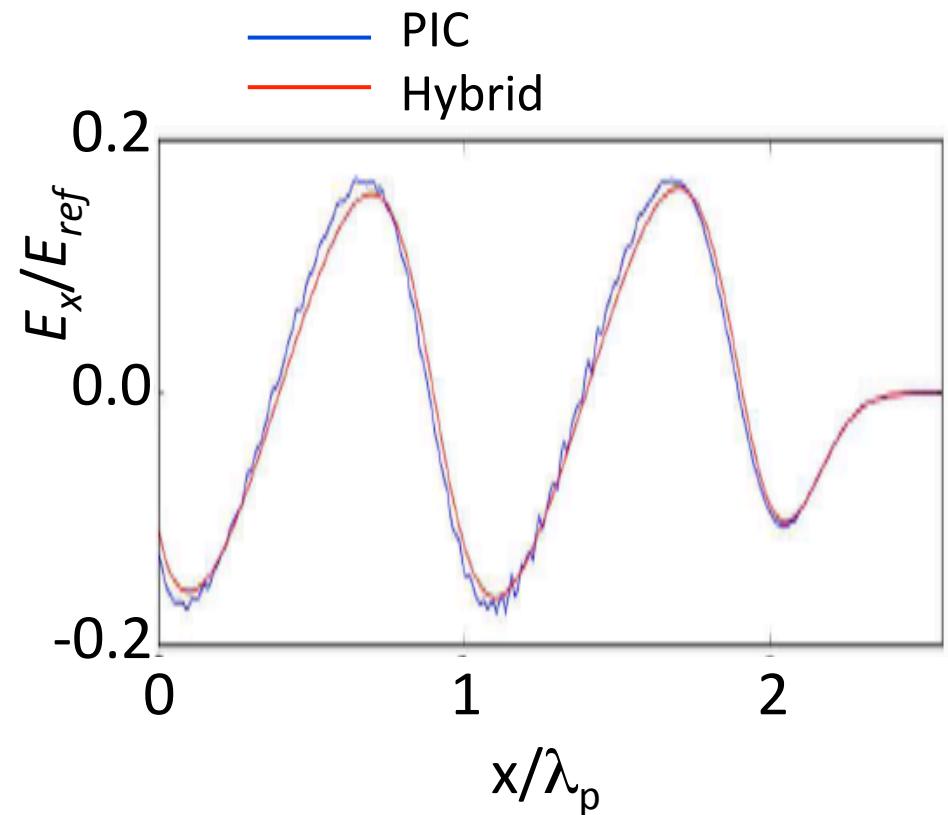
H-VLPL3D: New hybrid PIC-Fluid code*

Hybrid PIC-Fluid enables simulation of 100s of plasma oscillations w/ small losses.

PIC needs higher resolution (x64) to reach same level of accuracy

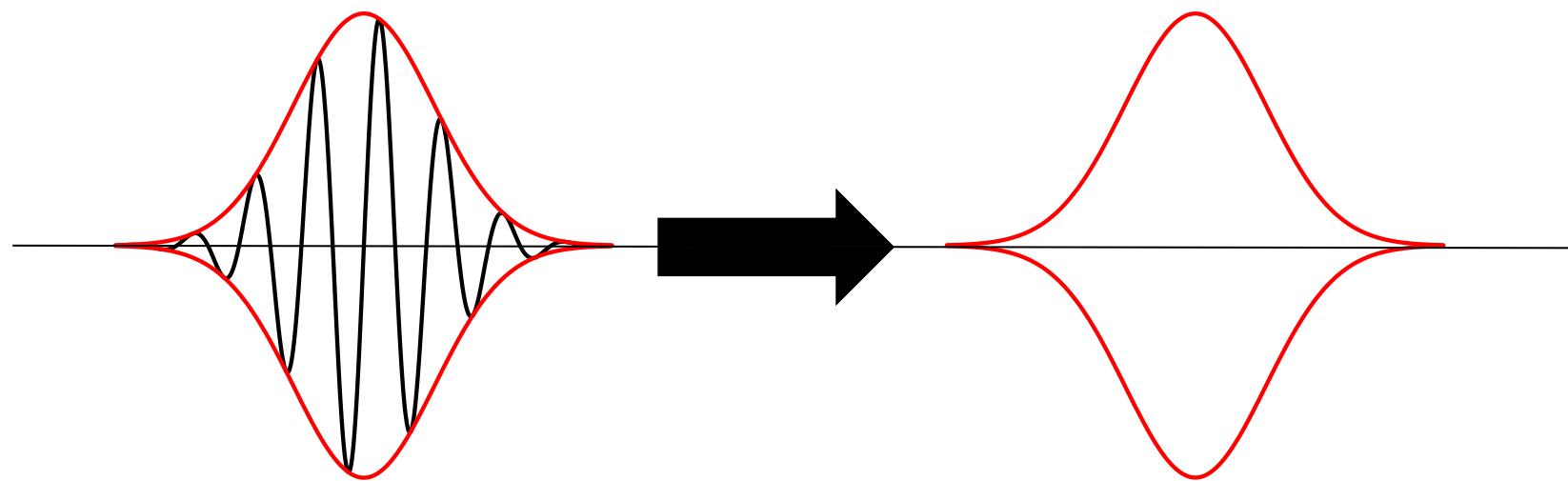


Hybrid PIC-Fluid is quieter



*T. Tuckmantel, A. Pukhov, J. Liljo, M. Hochbruck, *IEEE Trans. Plasma Science* **38**, 2383-2389 (2011)

Envelope solvers





R-Z Mode implemented in TurboWAVE*

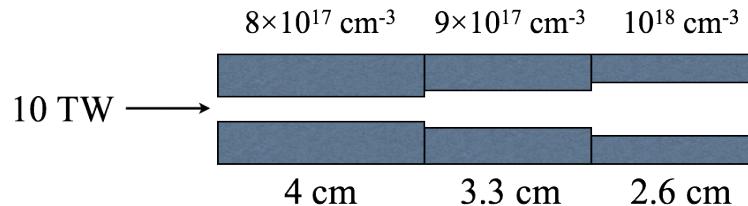
Plasma
Physics
Division



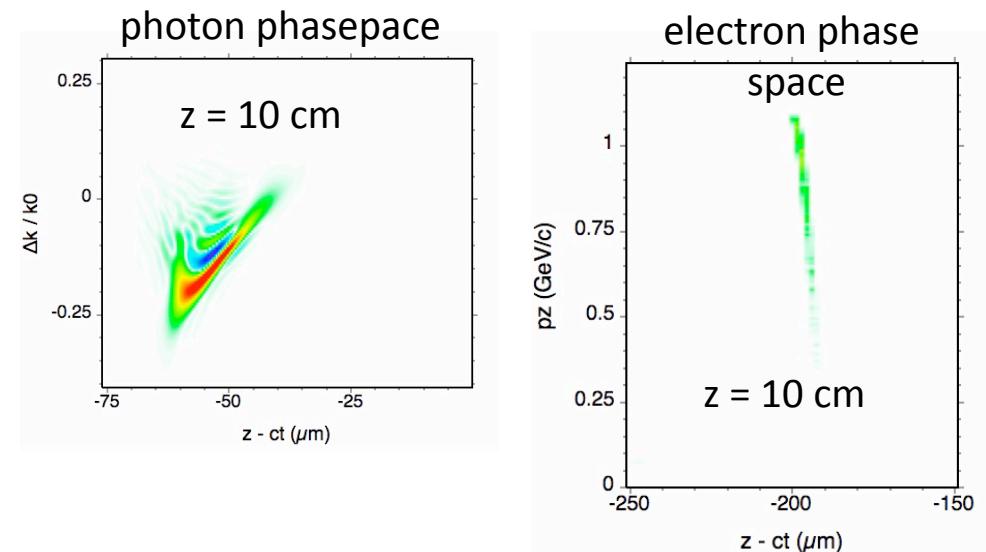
D.F. Gordon, A. Ting, M.H. Helle, D. Kaganovich, B. Hafizi, J.R. Penano, P. Sprangle, R.F. Hubbard, W.B. Mori, T.M. Antonsen, Jr.

- Averaging over laser cycles speeds calculation by $(\omega/\omega_p)^2$
- Full particle-wake dynamics are retained
- Envelope models take advantage of axisymmetry

Segmented-tapered capillary for enhanced electron acceleration



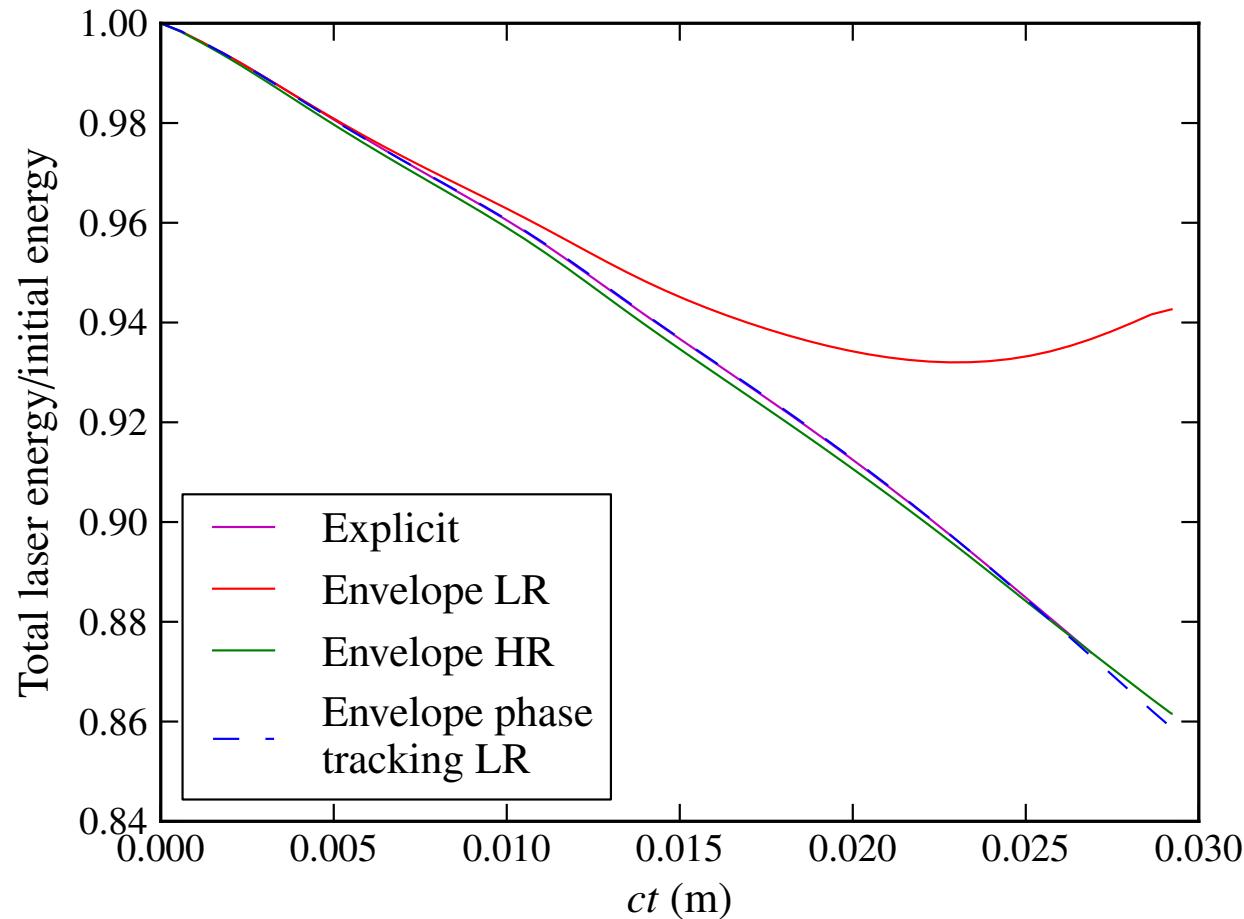
Full scale simulation
(~100 core-hours per cm)



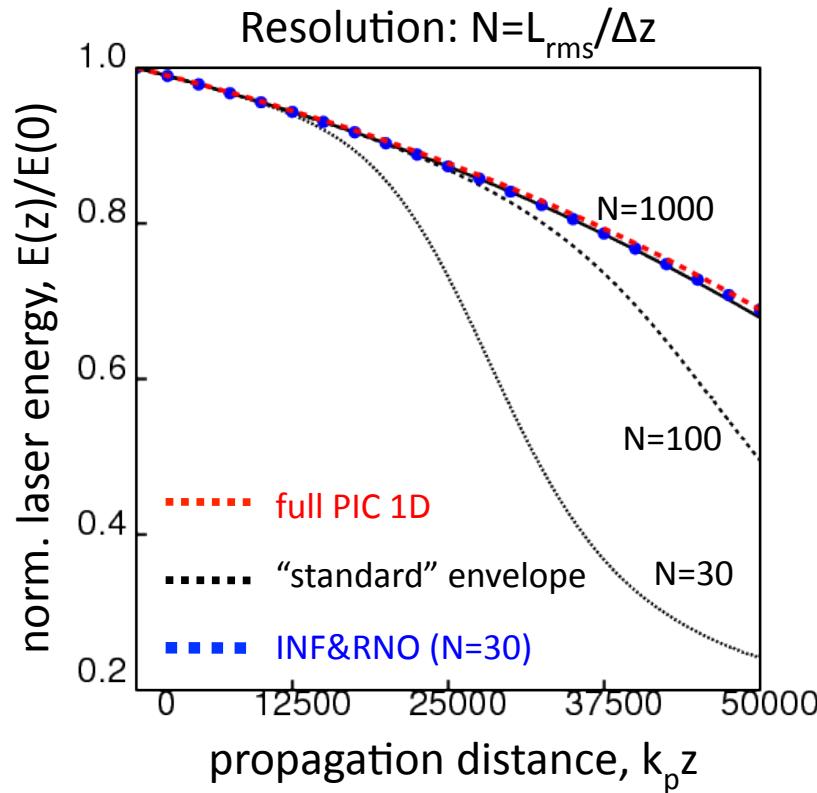
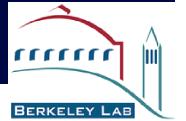
Obtained GeV using modest 10 TW

* D.F. Gordon et al., SPIE Optics+Optoelectronics 8079, 80790J (2011), D.F. Gordon, IEEE Trans. Plasma Sci. 35, 1486 (2007), D.F. Gordon et al., IEEE Trans. Plasma Sci. 28, 1224 (2000)

- Phase tracking included in Vorpal's envelope model*
 - successfully tested against HR runs for mildly depleted 100 MeV stage



INF&RNO*: new polar envelope solver superior to standard cartesian
 -- envelope + boosted frame → higher speedup



INF&RNO:

2D-RZ parallel PIC/fluid code

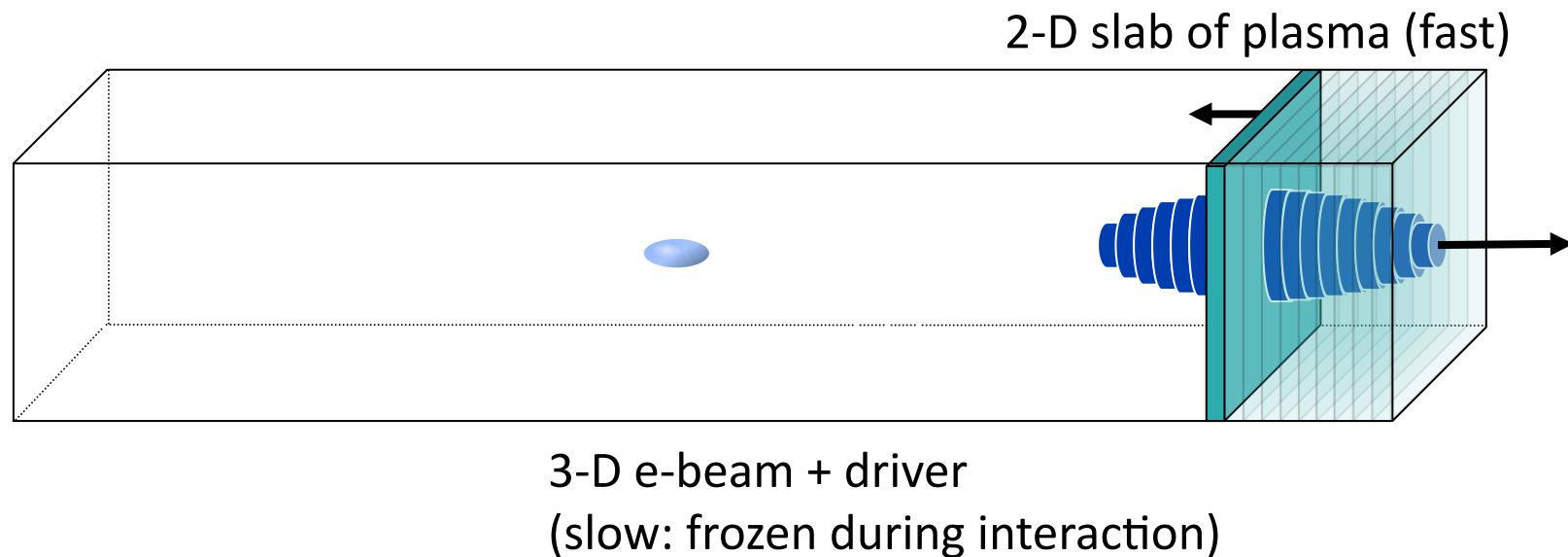
Test: $a_0=1$, $k_0/k_p=100$, $k_p L_{\text{rms}}=1$

Improved laser-envelope solver

- “polar” representation for complex laser amplitude \hat{a} [$\hat{a} = \text{Re}\{\hat{a}\} + i \text{Im}\{\hat{a}\} = |\hat{a}| \exp(i\theta)$]
- 2nd-order implicit Crank-Nicolson for FULL wave operator → enabling BLF simulations

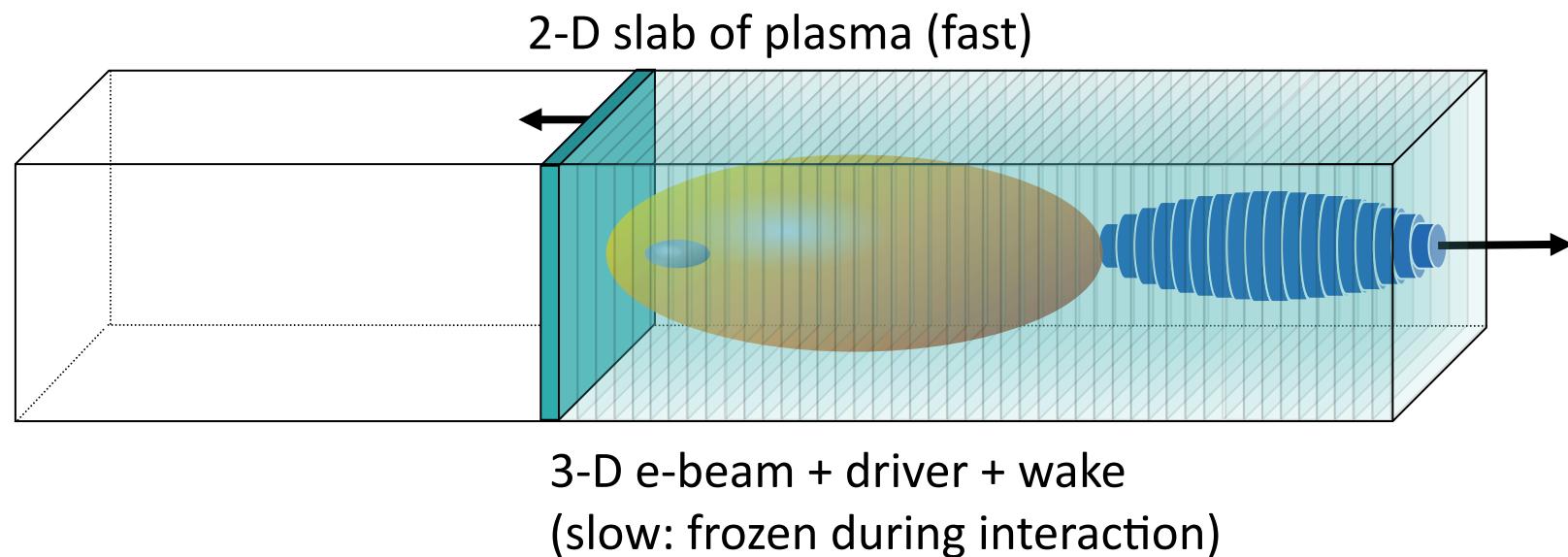
* Benedetti *et al.*, Proc. of AAC10 (2010)
 Benedetti *et al.*, Proc. of PAC11 (2011)¹⁵

Quasistatic* solvers



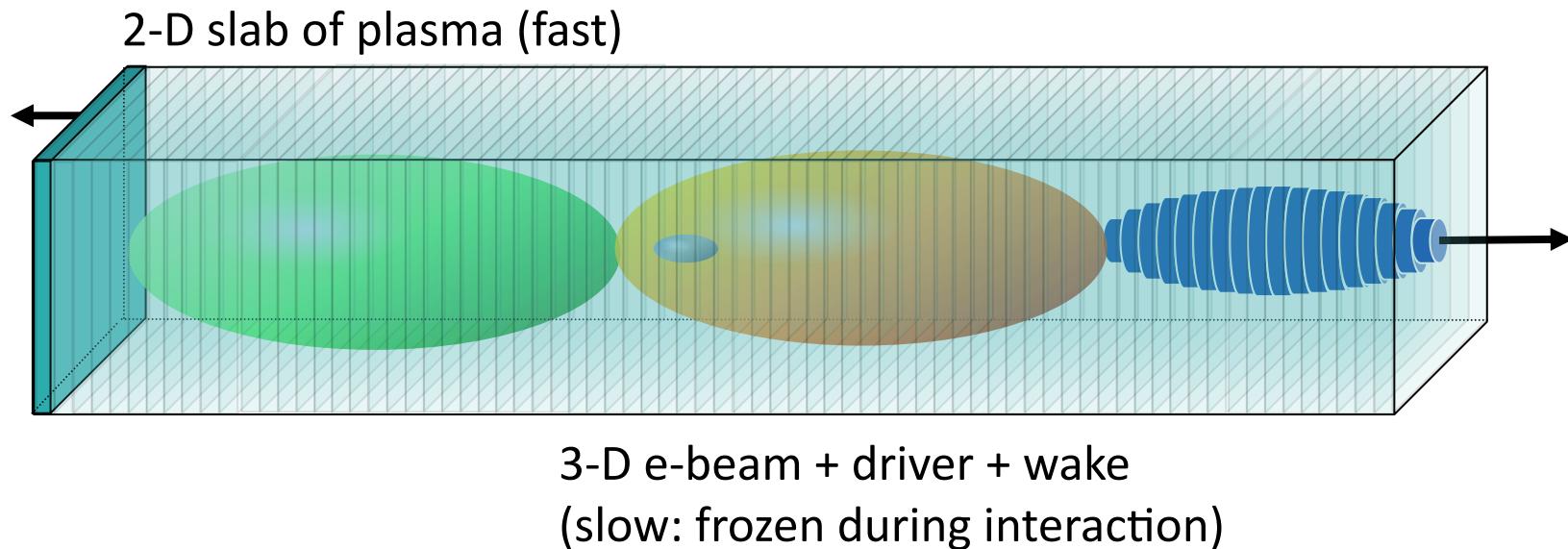
*P. Sprangle, E. Esarey and A. Ting, Phys. Rev. Lett. 64, 2011 (1990)

Quasistatic* solvers



*P. Sprangle, E. Esarey and A. Ting, Phys. Rev. Lett. 64, 2011 (1990)

Quasistatic* solvers



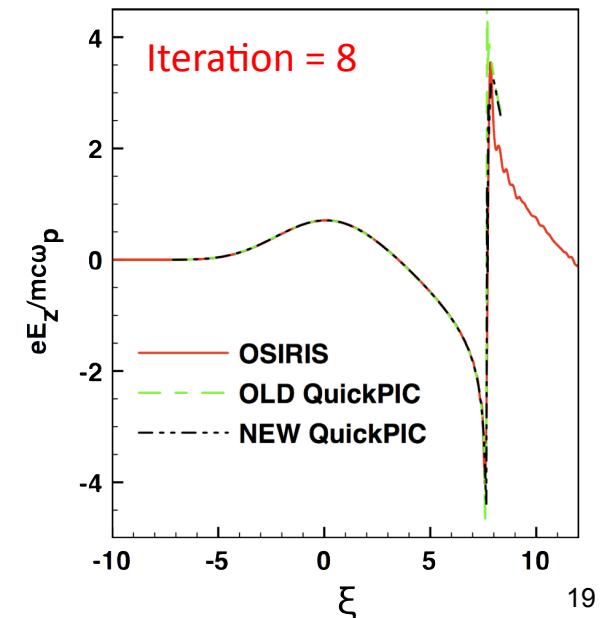
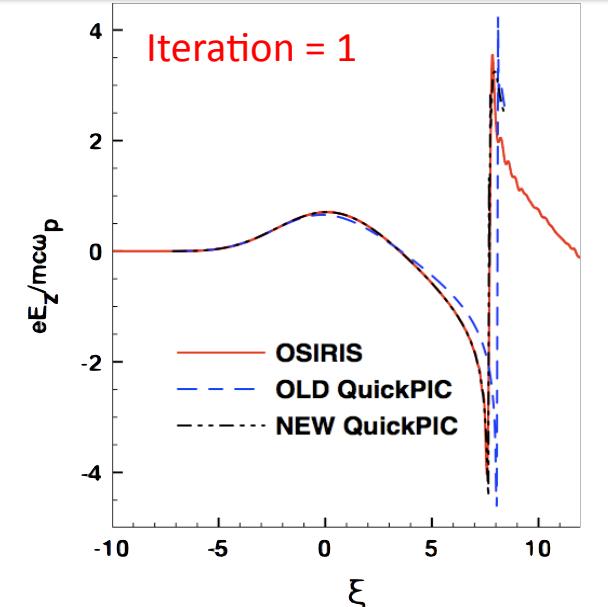
*P. Sprangle, E. Esarey and A. Ting, Phys. Rev. Lett. 64, 2011 (1990)

BEFORE

$$\begin{aligned}\frac{\partial \psi}{\partial \xi} &= -\nabla_{\perp} \cdot \vec{A}_{\perp} \\ \vec{J}_{\perp} &= -\nabla_{\perp}^2 \vec{A}_{\perp} \\ J_z &= -\nabla_{\perp}^2 A_z \\ \rho &= -\nabla_{\perp}^2 \phi\end{aligned}$$

NOW

$$\begin{aligned}\vec{E}_{\perp} + \hat{z} \times \vec{B}_{\perp} &= -\nabla_{\perp} \cdot \psi \\ \nabla_{\perp}^2 \psi &= -(\rho - J_z) \\ \nabla_{\perp}^2 \vec{B}_{\perp} &= \hat{z} \times \left(\frac{\partial}{\partial \xi} \vec{J}_{\perp} + \nabla_{\perp} \cdot J_z \right) \\ \nabla_{\perp}^2 B_z &= -\nabla_{\perp} \times \vec{J}_{\perp} \\ \nabla_{\perp}^2 E_z &= \nabla_{\perp} \cdot \vec{J}_{\perp}\end{aligned}$$



Electron beam driven wakefield in the blow-out regime

e⁻ beam: $\sigma_r = 1 \mu\text{m}$, $\sigma_z = 30 \mu\text{m}$, $N = 3.0 \times 10^{10}$, $\varepsilon_x = \varepsilon_y = 10 \text{ mm}\cdot\text{mrad}$
 Plasma density: $1.0 \times 10^{17} \text{ cm}^{-3}$

- accurate solution in a single iteration (2 to 7 before)
depending on intensity of drive beam
- computing time shortened by a factor of 2 or more

[1] C. Huang et al., J. Phys.: Conf. Ser. 46, 190 (2006).

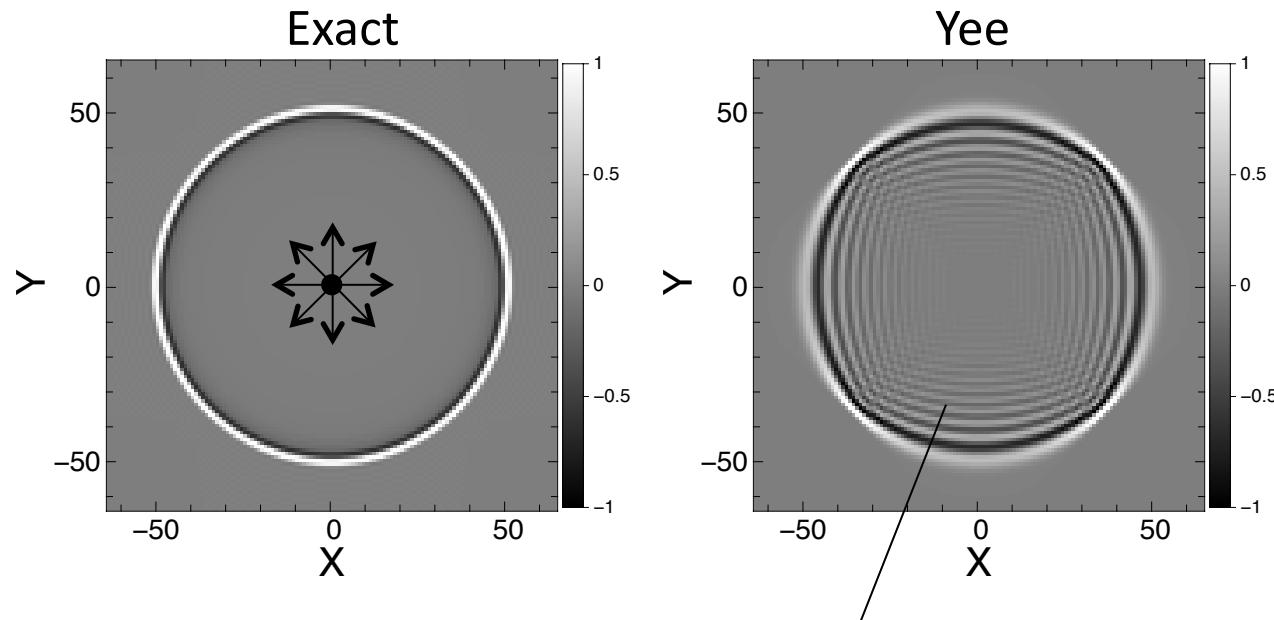
[2] V. K. Decyk, Computer Phys. Comm. 177, 95 (2007).

Full PIC

- NSFD electromagnetic solver
- Beam Frame Poisson Solver
- “strided” digital filtering

Yee field solver suffers from numerical dispersion errors

Expansion of a unit pulse



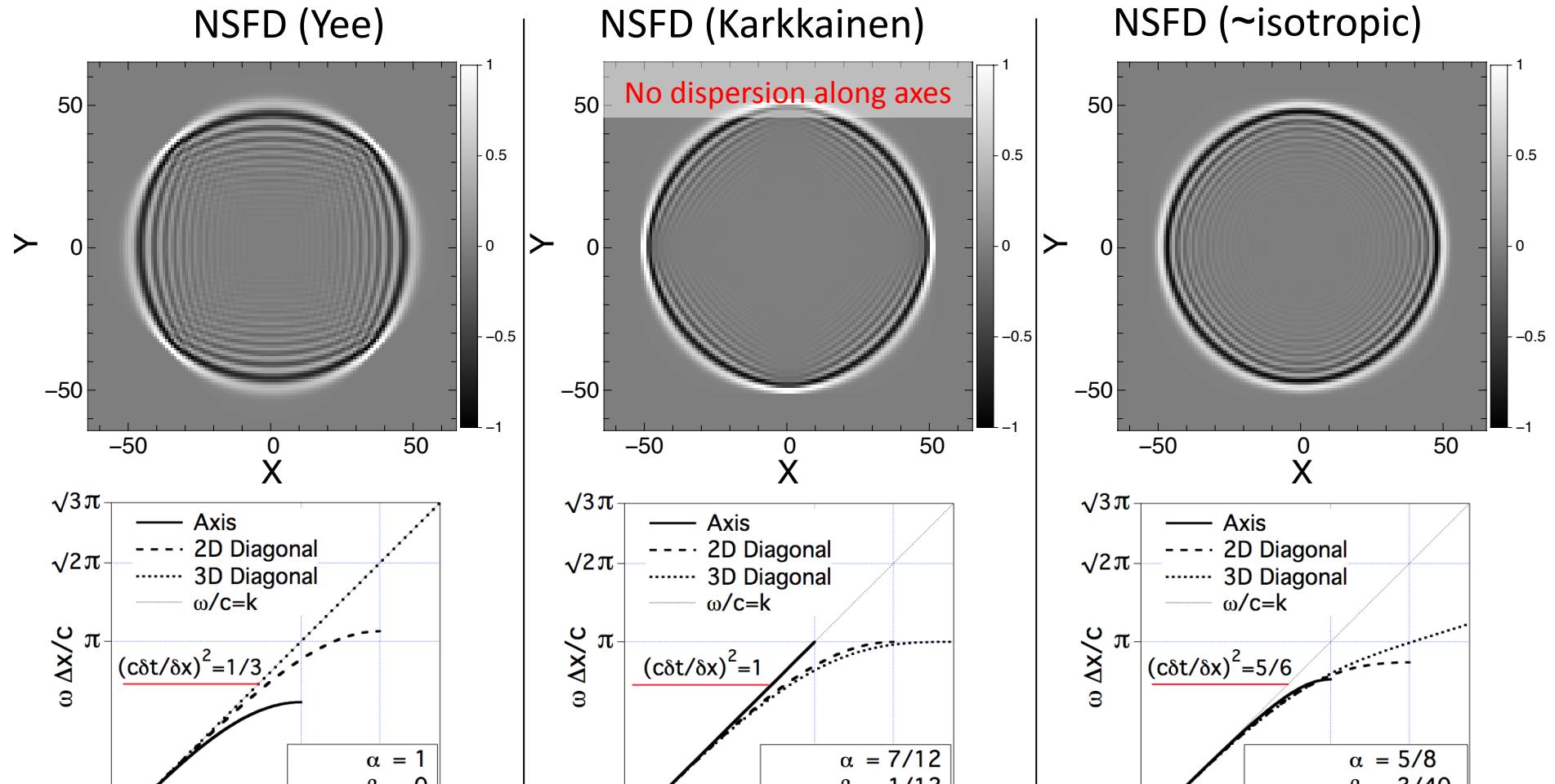
Numerical speed of short wavelength $< C$

- if relativistic particles \Rightarrow Numerical Cerenkov instability

Need for higher accuracy solver that blend adequately w/ standard PIC

Non-Standard Finite-Difference solver successfully blended with PIC¹

-- offers tunability of numerical dispersion



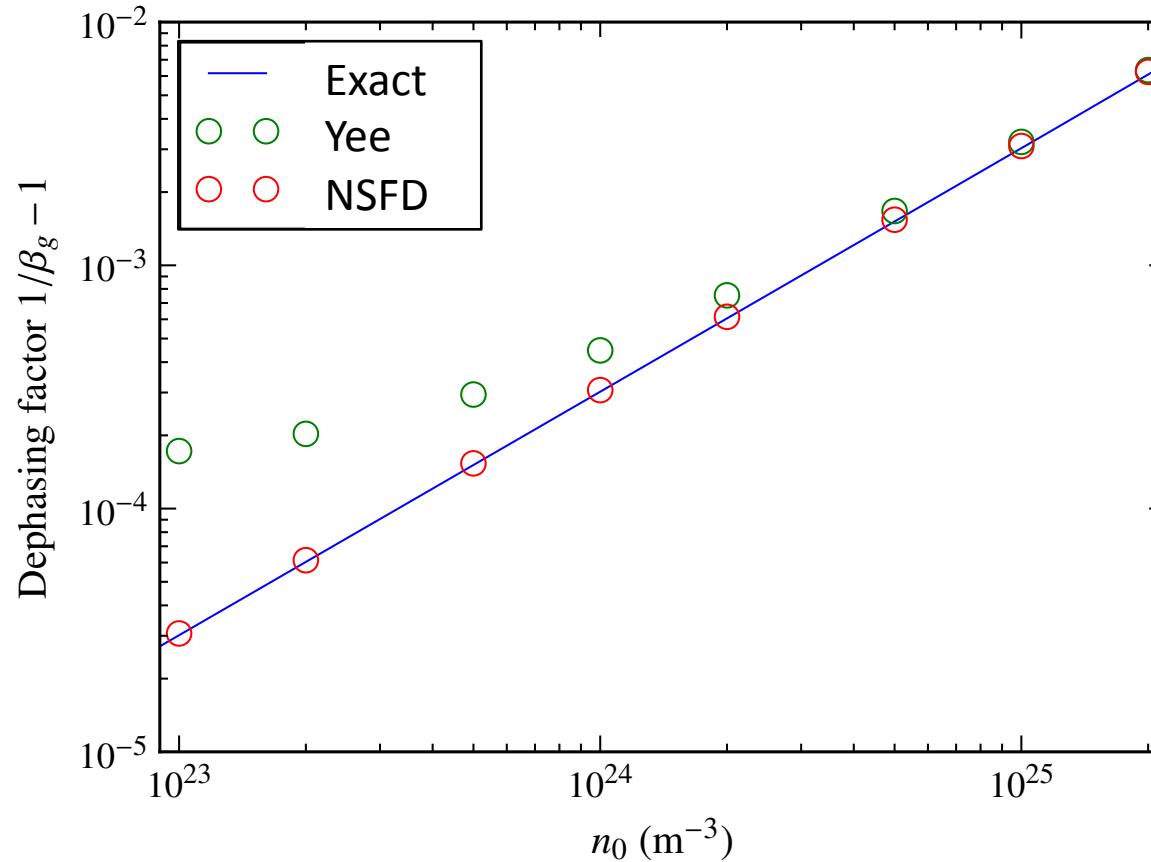
Note: NSFD (Karkkainen) solver is sometimes improperly referred to as “dispersionless” or “perfect dispersion” solver.

NSFD Maxwell solver implemented in Warp¹, Vorpal and Osiris.

¹J.-L. Vay, et al., *J. Comput. Phys.* **230** (2011).

²M. Karkkainen et al., Proc. ICAP, Chamonix, France (2006).

Improved dispersion enables correct group velocity, and hence dephasing

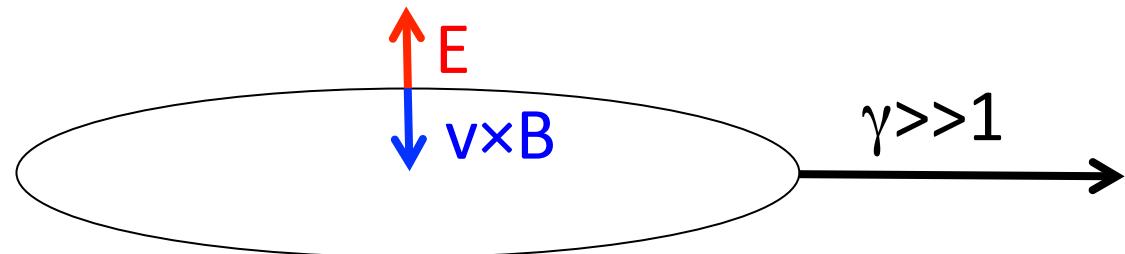


- Observed that accurate dephasing makes difference in injection simulations
- Further analysis underway

Standard PIC method inadequate for ultra-relativistic beams

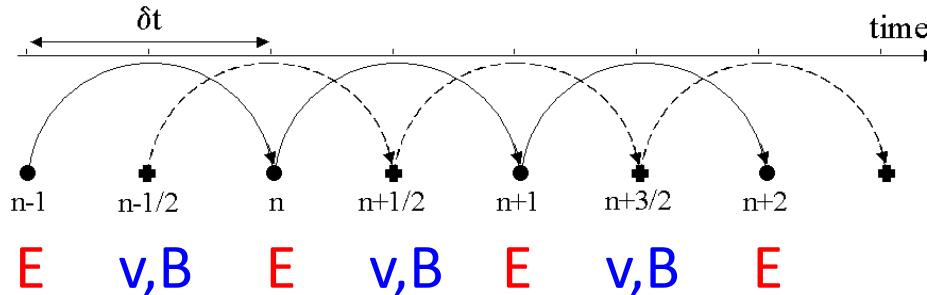
$\gamma \gg 1$: **exact cancellation** of self E and B contributions in Lorentz force

$$F = q(E + v \times B)$$

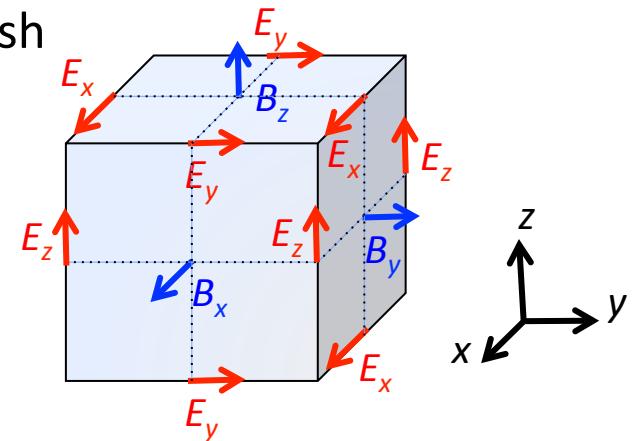


Spatial/time staggering in Boris/Yee pusher \rightarrow interpolation errors

Boris pusher

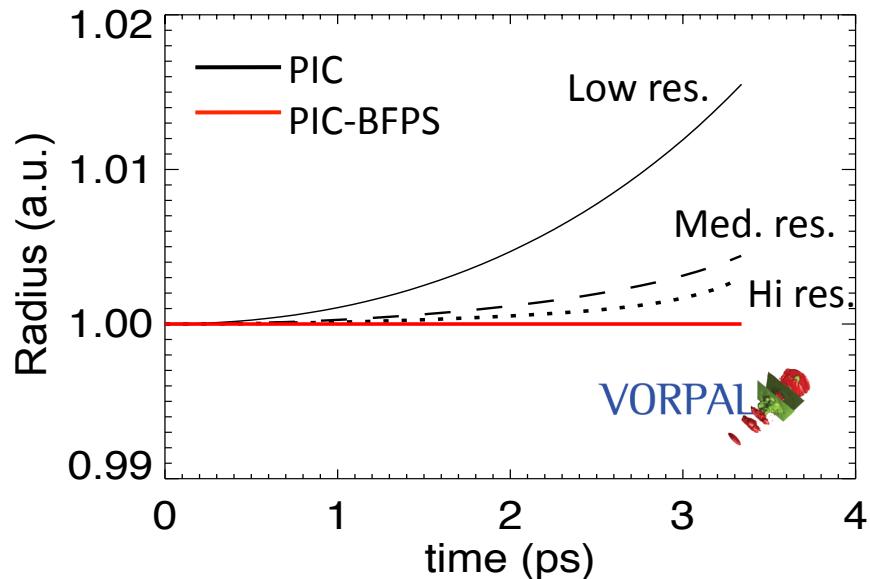


Yee mesh



Fix to Boris \rightarrow Lorentz invariant particle pusher: J.-L. Vay, *Phys. Plasmas* **15**, 056701 (2008)

Beam Frame Poisson Solver (BFPS) mitigates interpolation errors in Vorpal LPA simulations



Validated on simulation of matched e- beam in continuous focusing channel.

Is being applied to the modeling of LPA

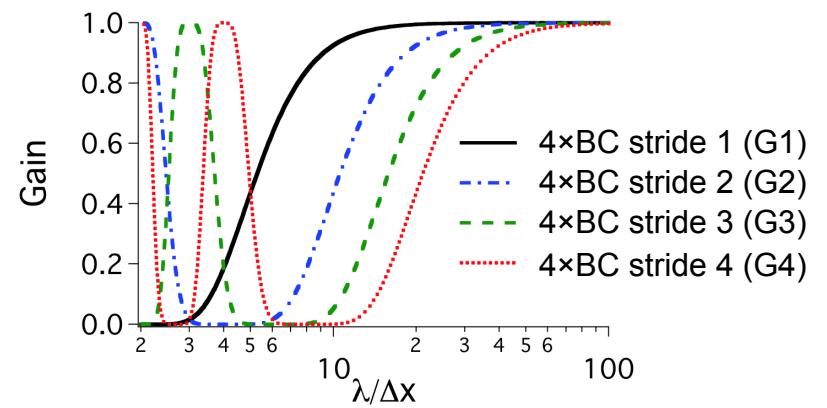
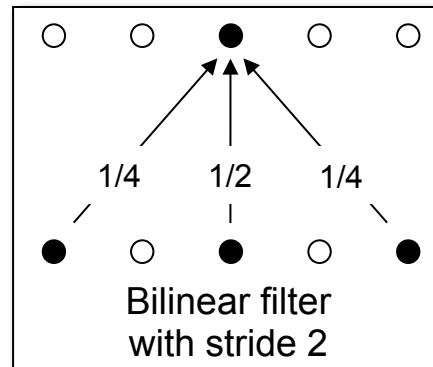
Electron bunch self-fields:

- E calculated approximately in beam-frame Poisson solve + $E = -\nabla \phi$,
- E Lorentz transformed to E', B' in the lab frame,
- E' & B' added to the plasma EM fields.

See talk from E. Cormier-Michel (WG2)

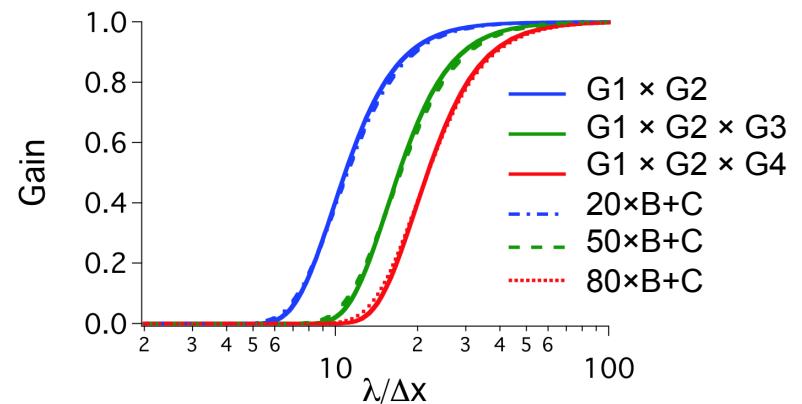
“Strided” bilinear filters enable more efficient filtering*

Using a stride N shifts the 100% absorption frequency to F_{nyquist}/N



Succession of passes with different strides → wideband filter:

- $G_1 G_2 \approx 20^* B+C$; speedup $\times 2$
- $G_1 G_2 G_3 \approx 50^* B+C$; speedup $\times 3.5$
- $G_1 G_2 G_4 \approx 80^* B+C$; speedup $\times 5.5$

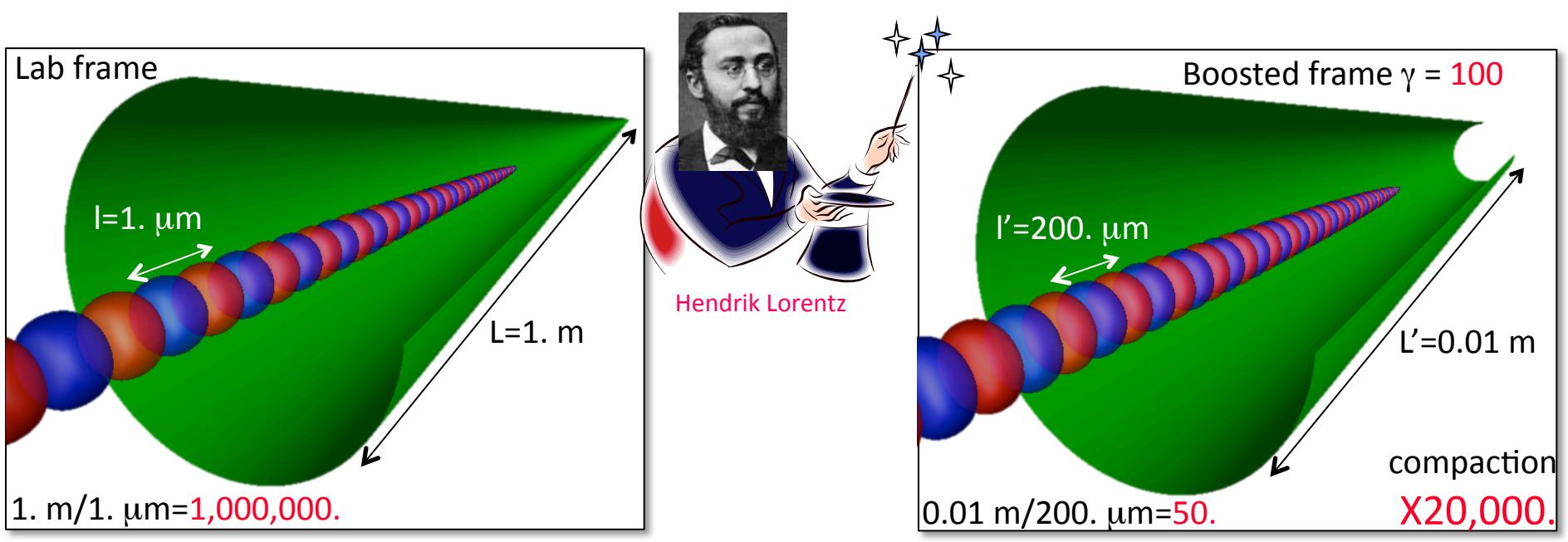


81 pass standard wideband filter down to 15 passes with strided filters

*J.-L. Vay, et al., *J. Comput. Phys.* **230**, 5908 (2011).

Lorentz boosted frame (LBF)

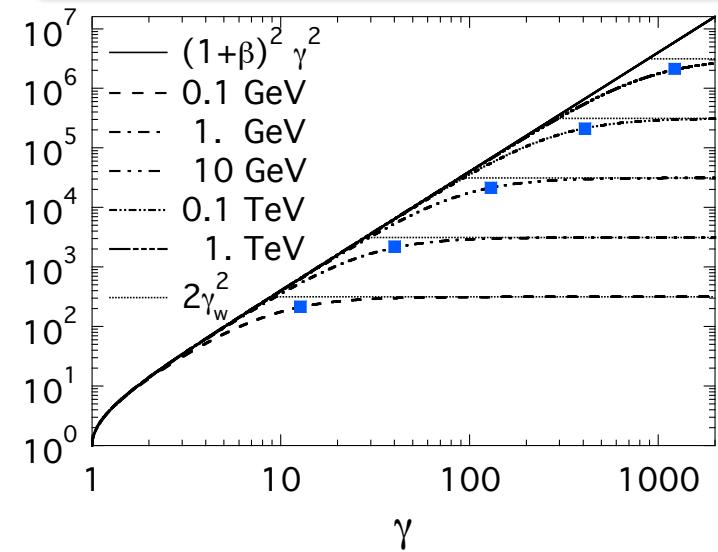
Lorentz boosted frame reduces scale range by orders of magnitude¹



LBF predicted speedup^{1,2}:

- > 10,000 for single 10 GeV (Bella) stage,
- > 1,000,000 for single 1 TeV stage.

Speedup



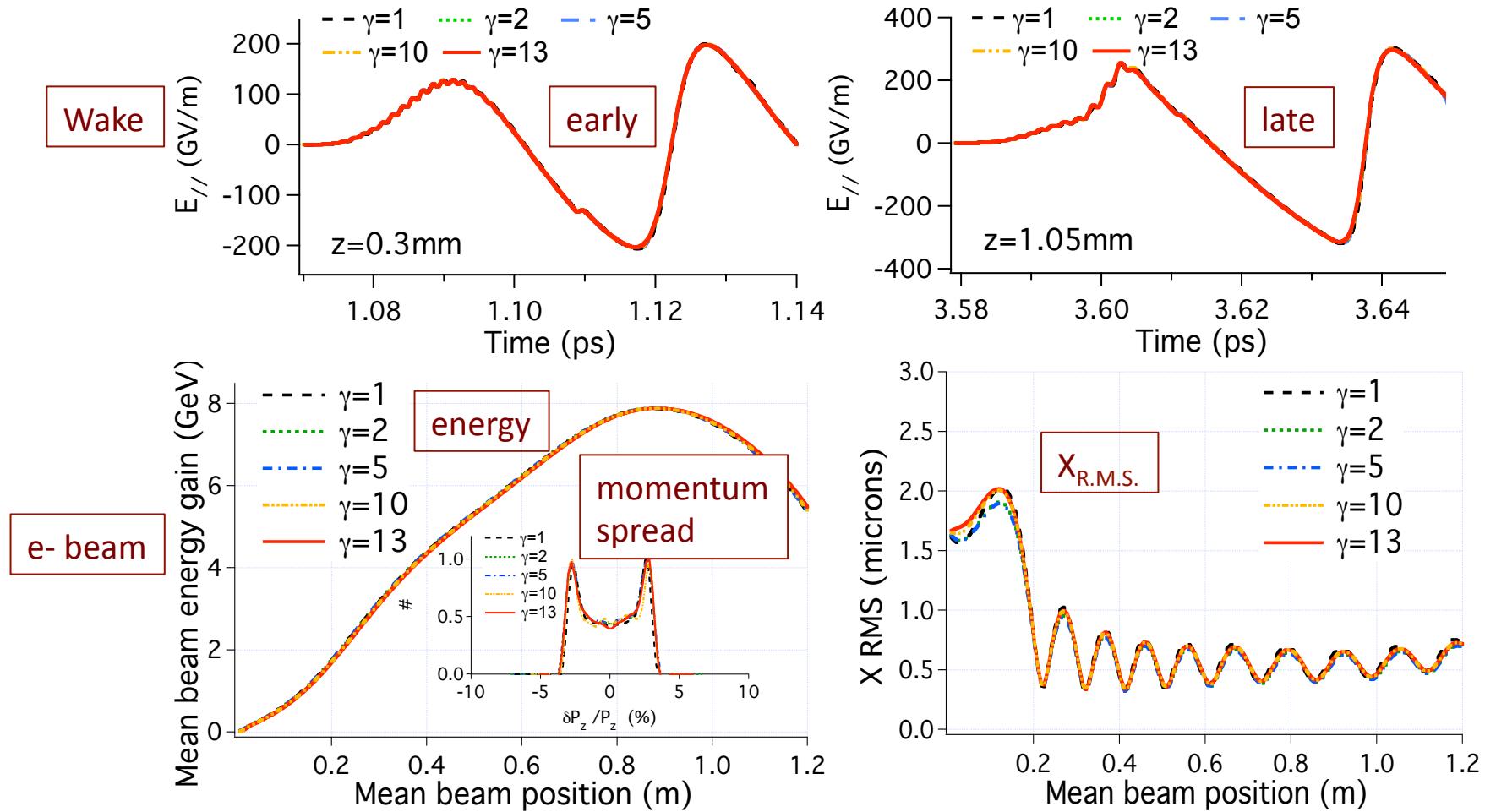
¹J.-L. Vay, *Phys. Rev. Lett.* **98**, 130405 (2007)

²J.-L. Vay, et al., *Phys. Plasmas* **18**, 123103 (2011)

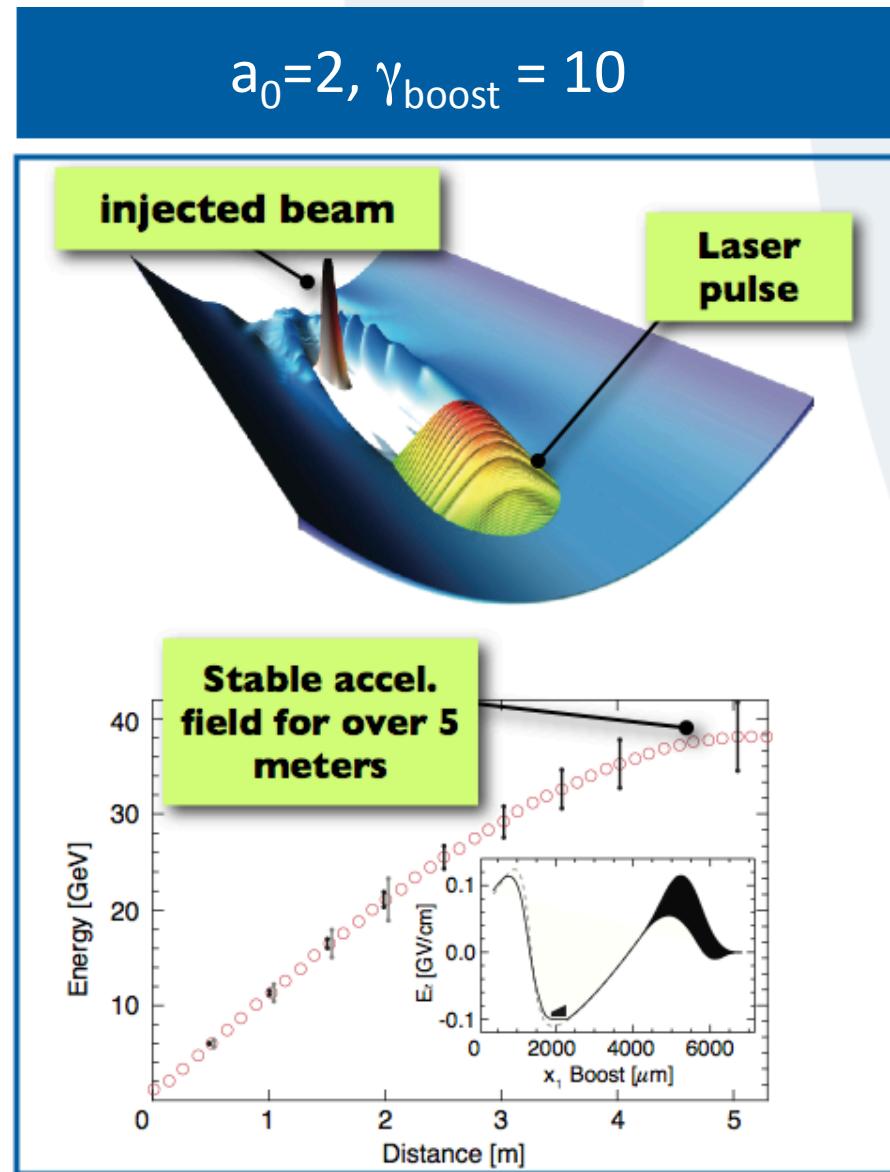
LBF method carefully validated in deeply depleted beam loaded stages

-- Excellent agreement between runs at various γ boost

Warp-3D – $a_0=1$, $n_0=10^{19}\text{cm}^{-3}$ ($\sim 100 \text{ MeV}$) scaled to 10^{17}cm^{-3} ($\sim 10 \text{ GeV}$)



Boosted frame* simulations with OSIRIS -- moderate blowout regime w/ external injection

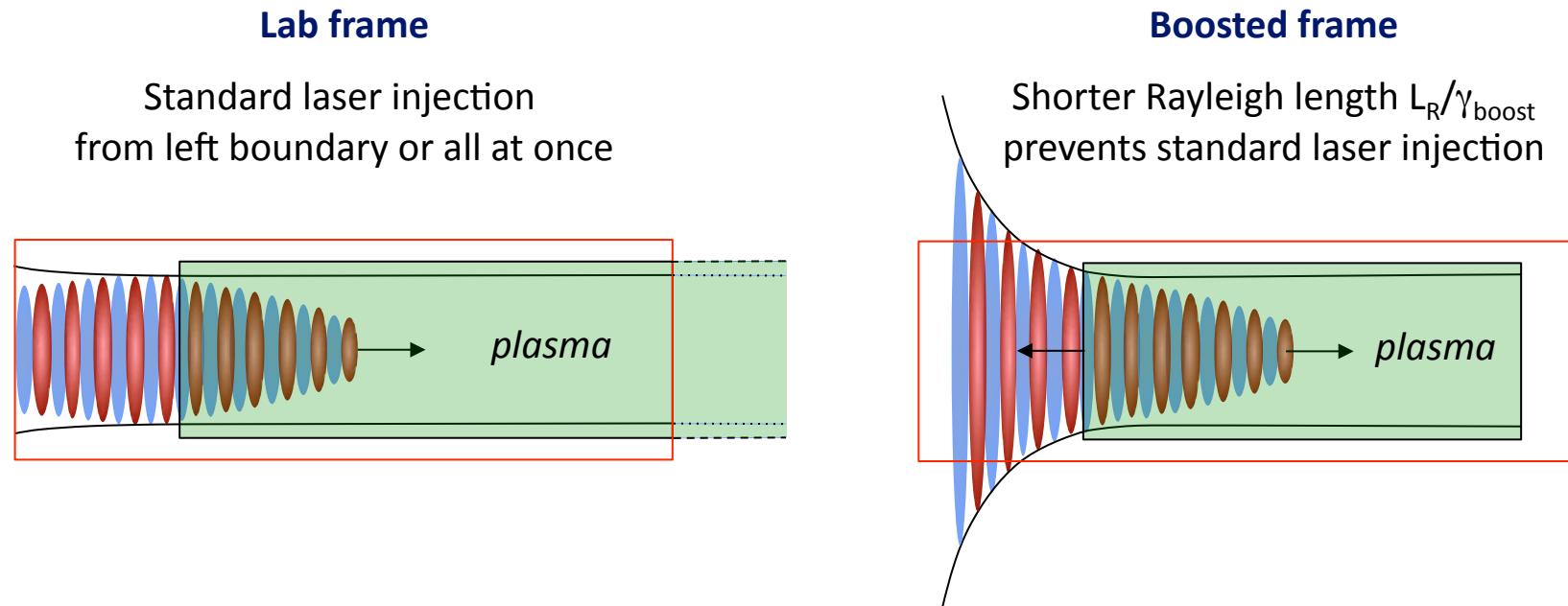


*J.-L. Vay, Phys. Rev. Lett. **98**, 130405 (2007)

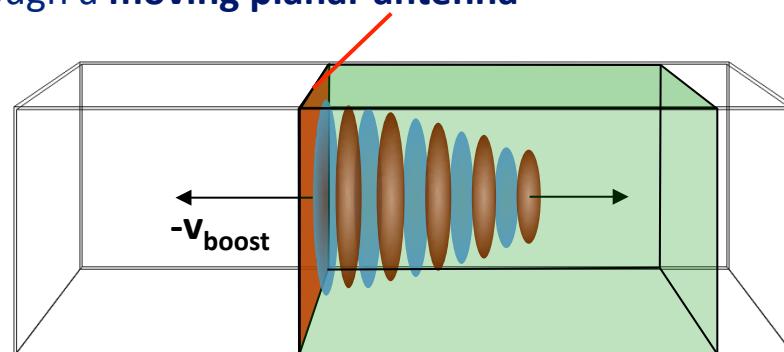
But two difficulties were identified at high γ boost:

- relative shortening of Rayleigh length complicates laser injection,
- instability developing at entrance of plasma.

Laser injection through moving plane solves initialization issue in LBF



Solution: injection through a **moving planar antenna** in front of plasma*

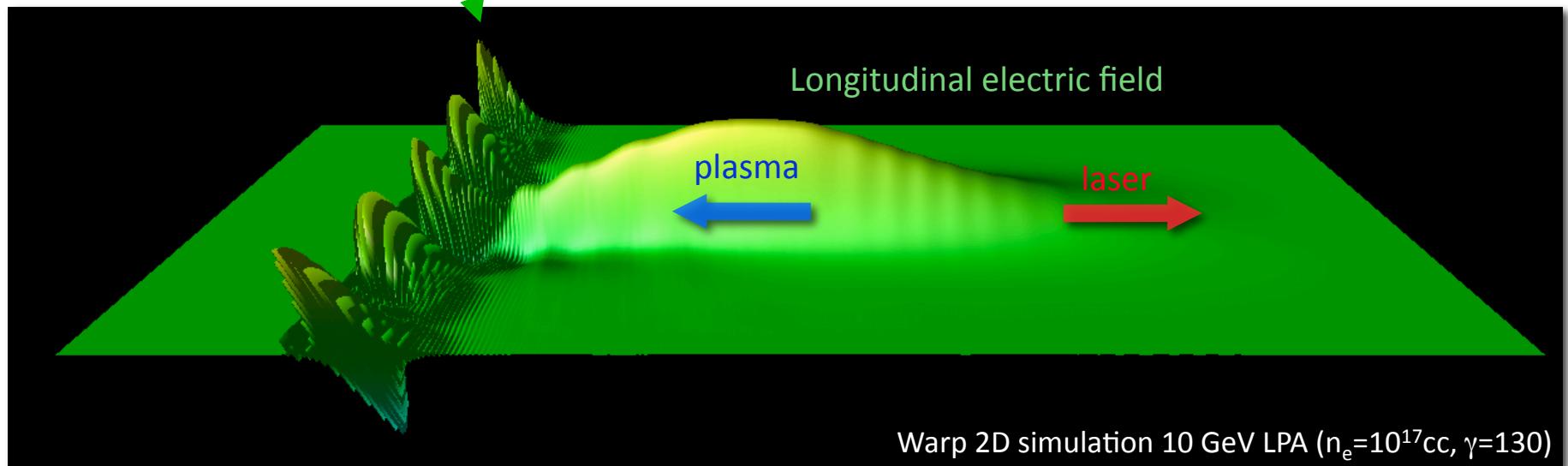


- Laser injected using macroparticles using Esirkepov current deposition ==> verifies Gauss' Law.
- For high γ_{boost} , backward radiation is blue shifted and unresolved.

Method has been developed in Warp*, and implemented in Osiris and Vorpal.

*J.-L. Vay, et al., *Phys. Plasmas* **18**, 123103 (2011)

Short wavelength instability observed at entrance of plasma for large γ (≥ 100)



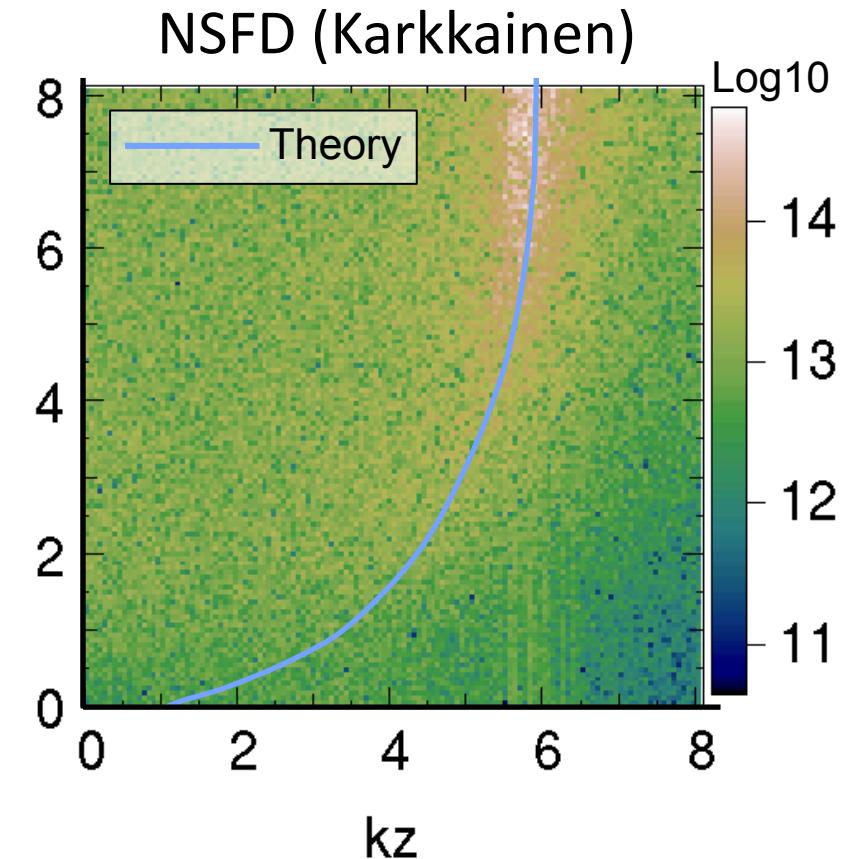
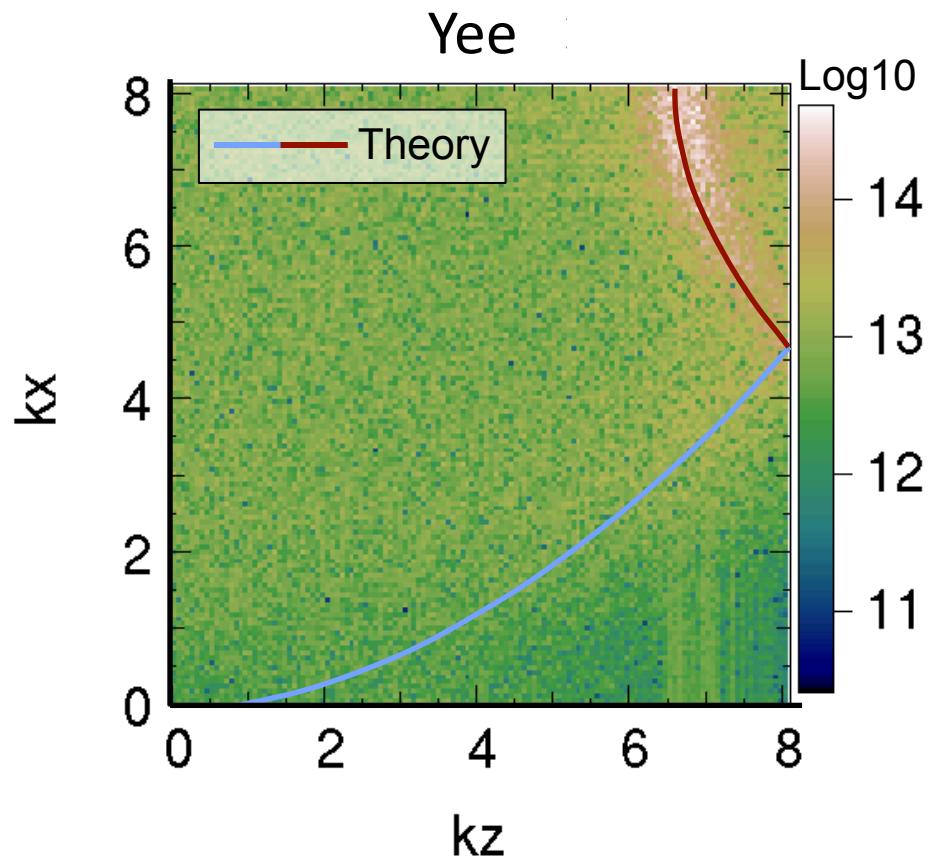
Is it Numerical Cerenkov? Other?

Study on nature of instability is underway

Qualitative agreement between simulation and theory but still incomplete understanding

At Berkeley Lab/U. Maryland (collaboration with B. Godfrey)

Comparison between theory and Warp simulations for the k-spectra transverse field



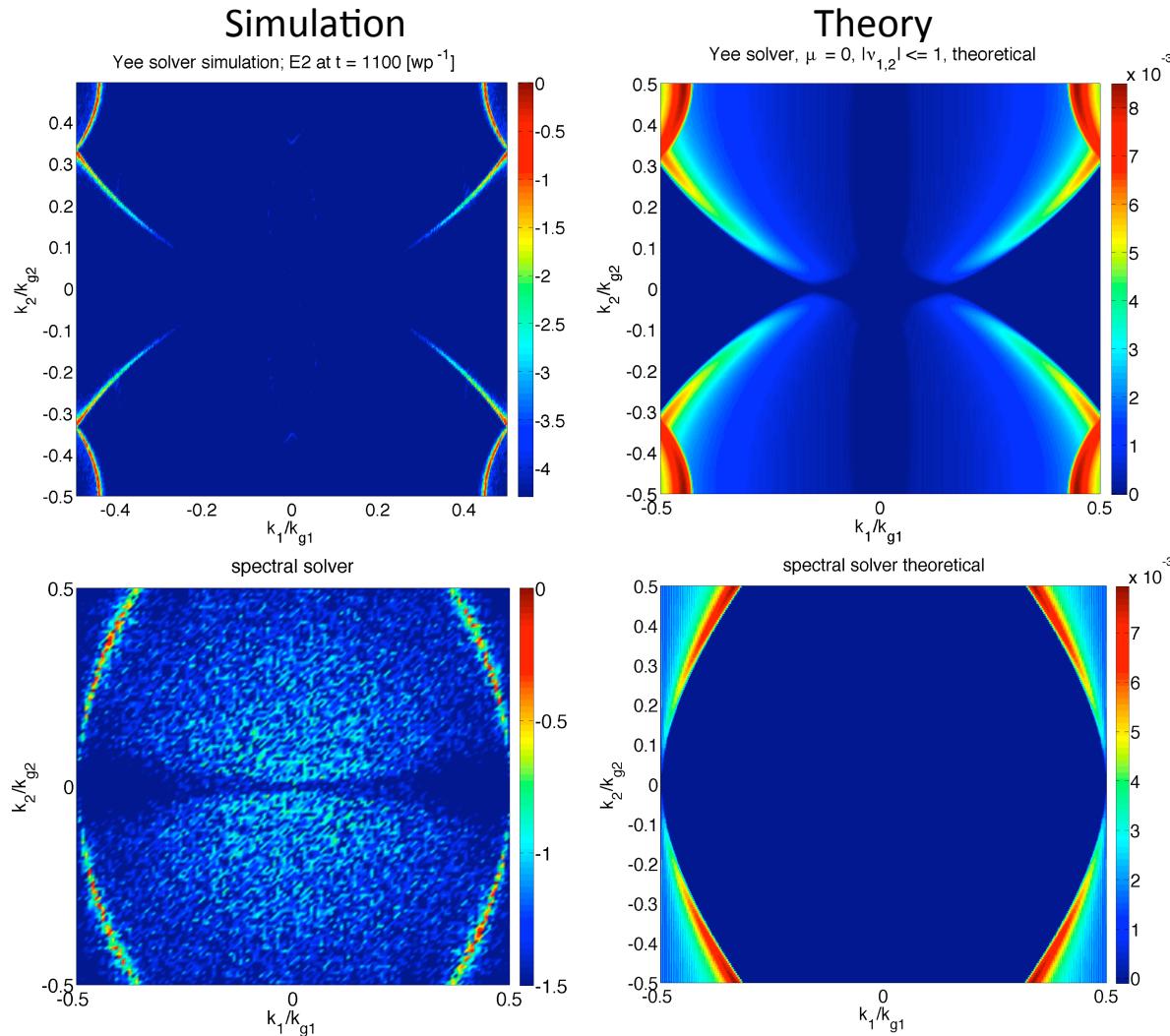
Study on nature of instability is underway - 2

Qualitative agreement between simulation and theory but still incomplete understanding

And at UCLA/IST - see talk from P. Yu (WG2)

Comparison between theory and Warp simulations for the k-spectra transverse field

Yee Mesh



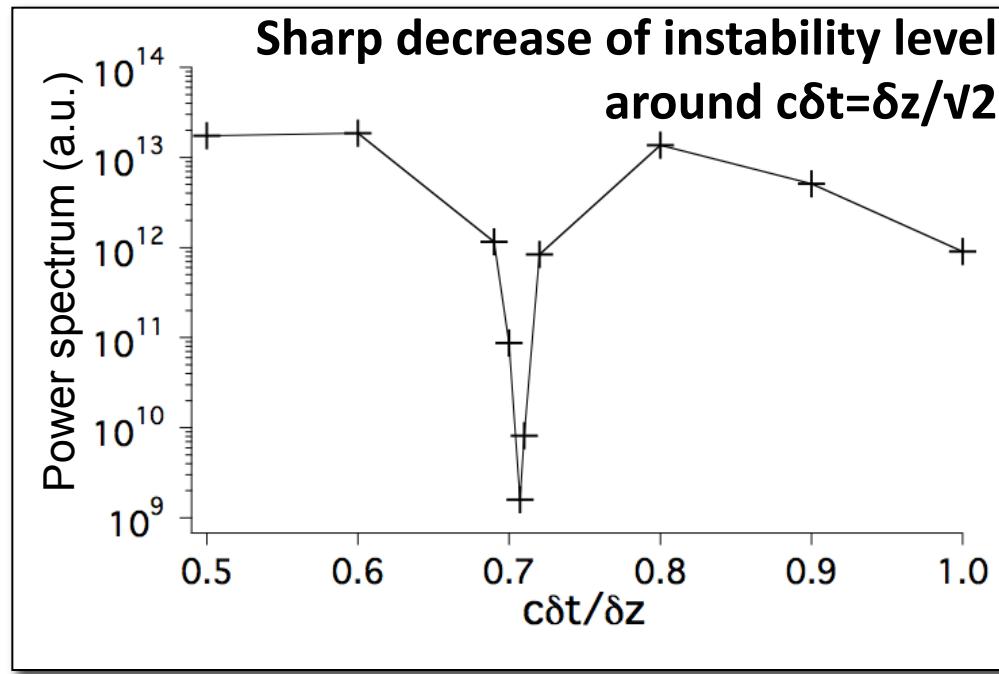
Spectral solver

Instability not yet understood, but can it be mitigated with:

- NSFD (Karkkainen) solver with no numerical dispersion along axes?
- wideband digital filtering?
- other trick?

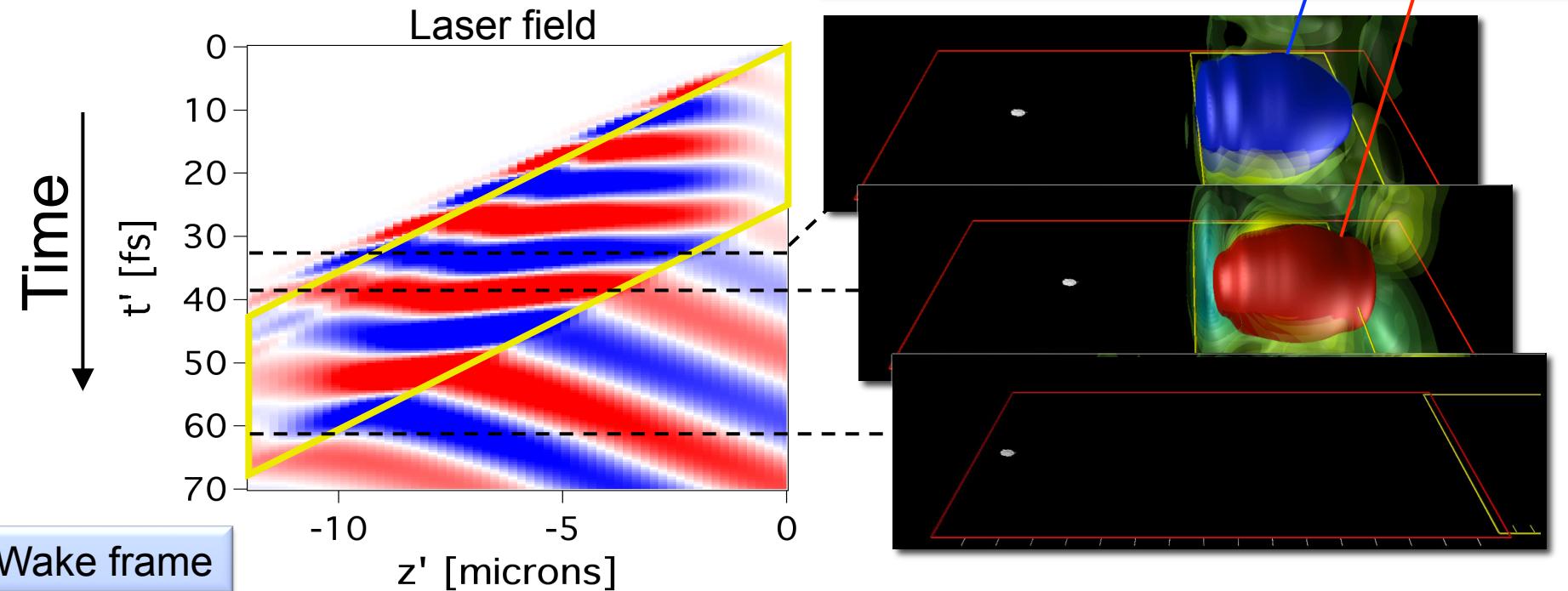
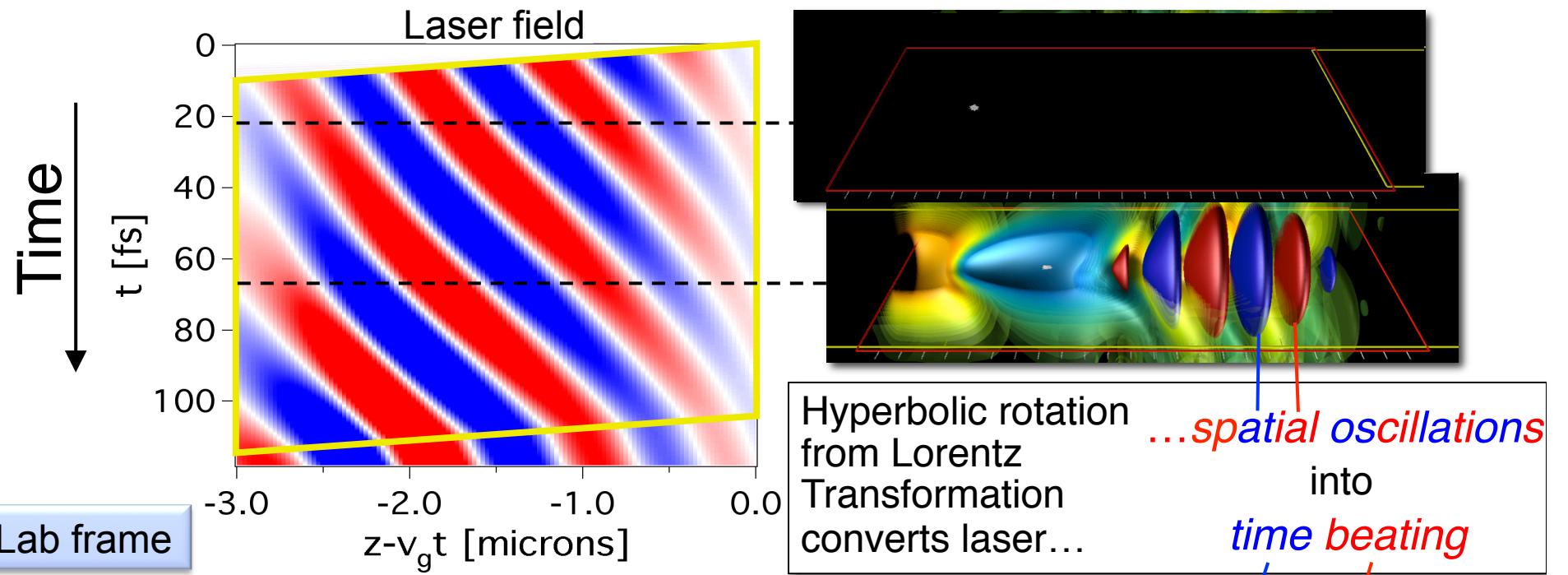
Comparing runs using Yee or NSFD (Karkkainen) solvers revealed

Instability mostly insensitive to tuning of numerical dispersion...
...but **very sensitive to time step***!



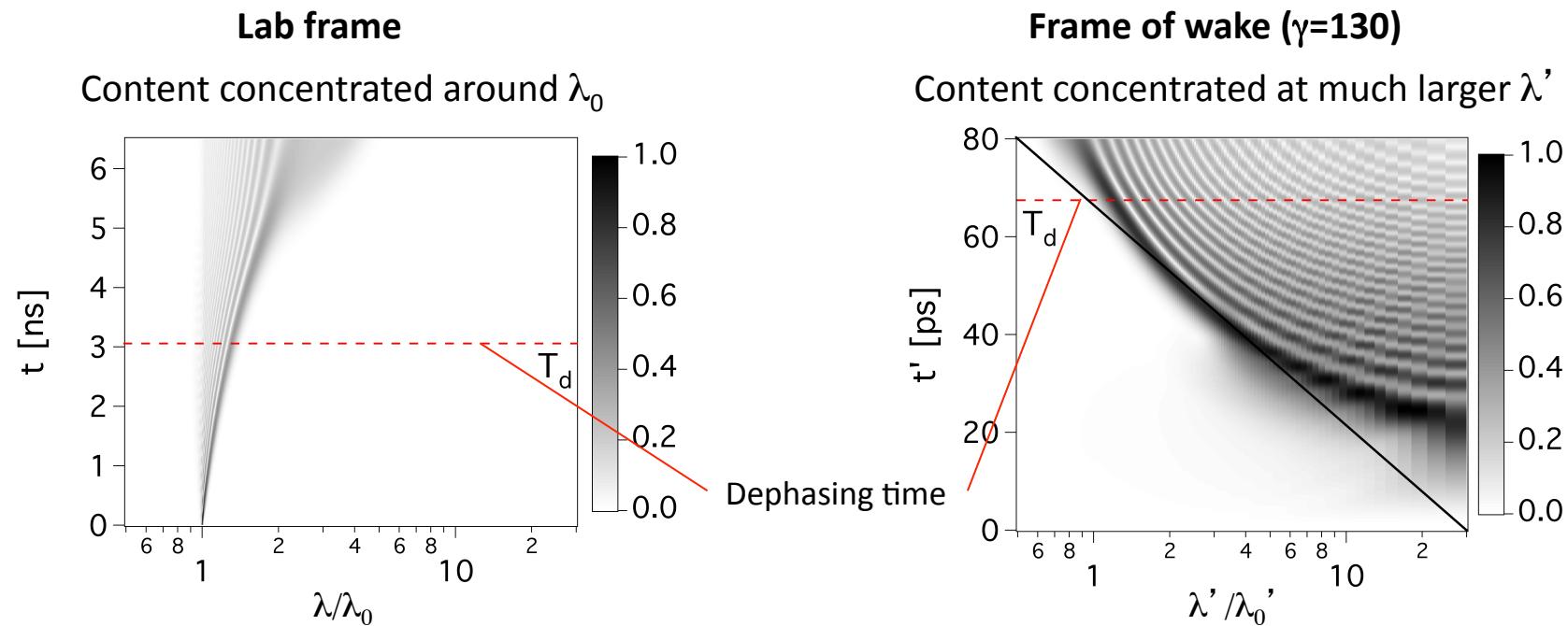
- Tunable NSFD solver enables $c\delta t = \delta z/\sqrt{2}$ time step for cubic cells
- Use of special time step is very beneficial but not sufficient for very large γ boost
→ need for wideband filtering

*J.-L. Vay, et al., *J. Comput. Phys.* **230**, 5908 (2011).



Spectrum very different in lab and boosted frame
 -- wideband filtering possible in wake frame without altering physics

Time history of laser spectrum (relative to laser λ_0 in vacuum)



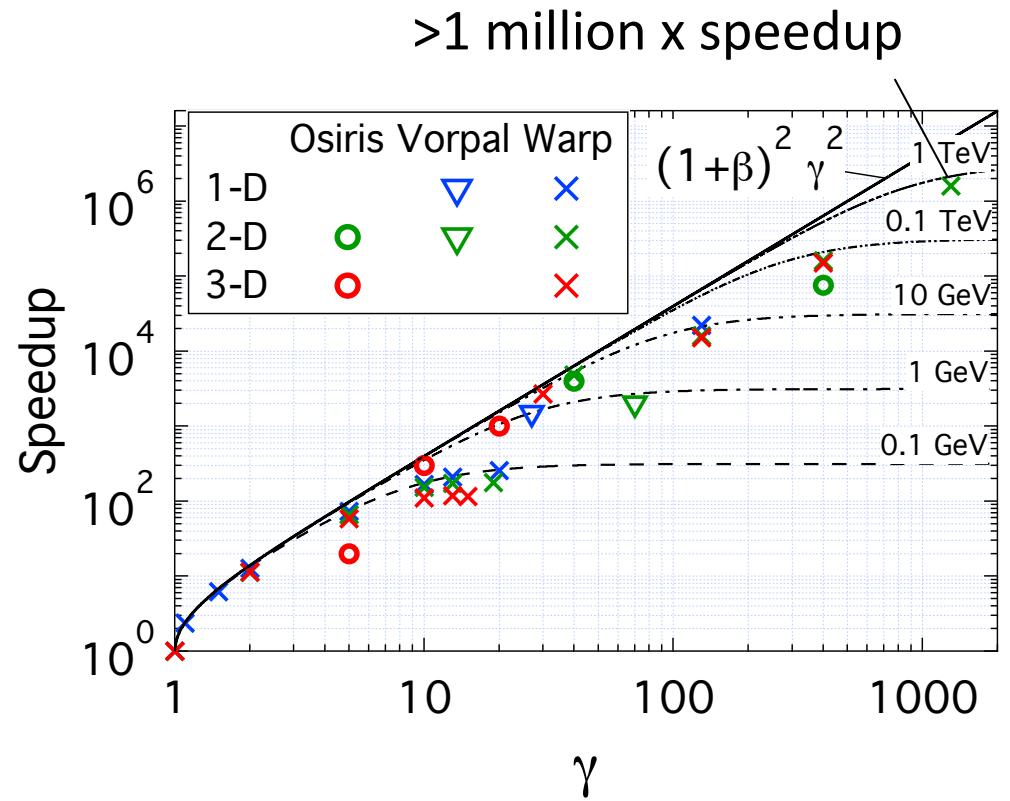
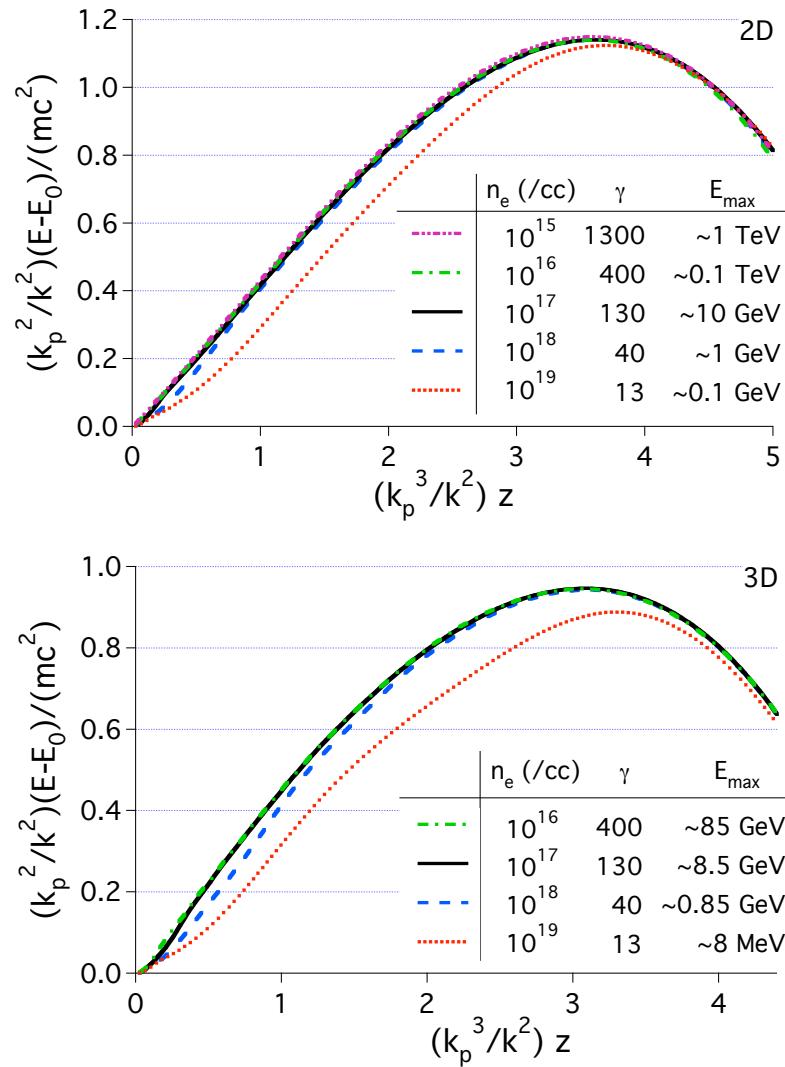
Spectrum very different in lab and boosted frames*:

→ wideband filtering possible in wake frame without altering physics!

*J.-L. Vay, et al., *Phys. Plasmas* **18** (2011).

- Planar antenna for laser injection
 - Control of instability
- full realization of BF speedup potential

Enabled verification of scaling of up-to 1 TeV (2D), \sim 100 GeV (3D), $a_0=1$
-- reaching >1 million x speedup for 2D 1TeV stage



Full PIC simulations of LPA:

2006 (lab): 10 GeV in 1D $\sim 5k$ CPU-hours

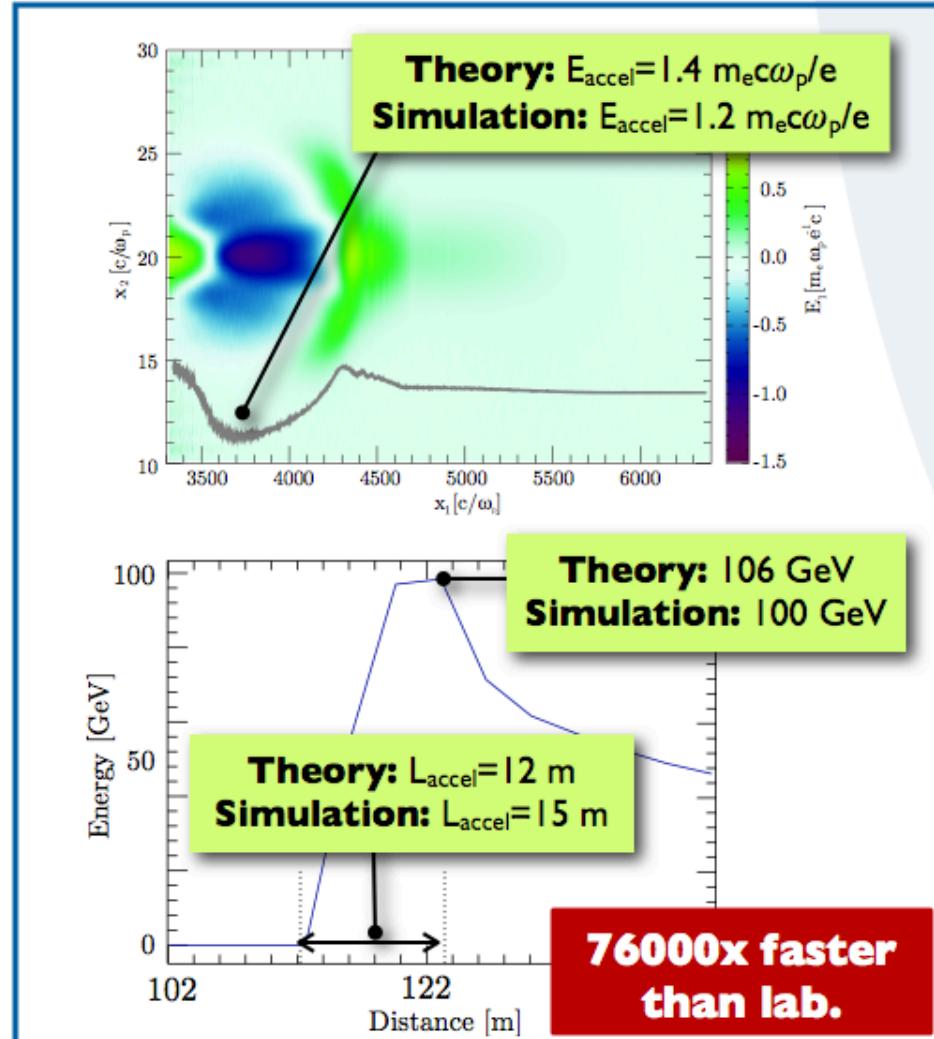
2011 (boost): 100 GeV in 3D $\sim 10k$ CPU-hours

LWFA modeling up to 100 GeVs with Osiris – $a_0=2$

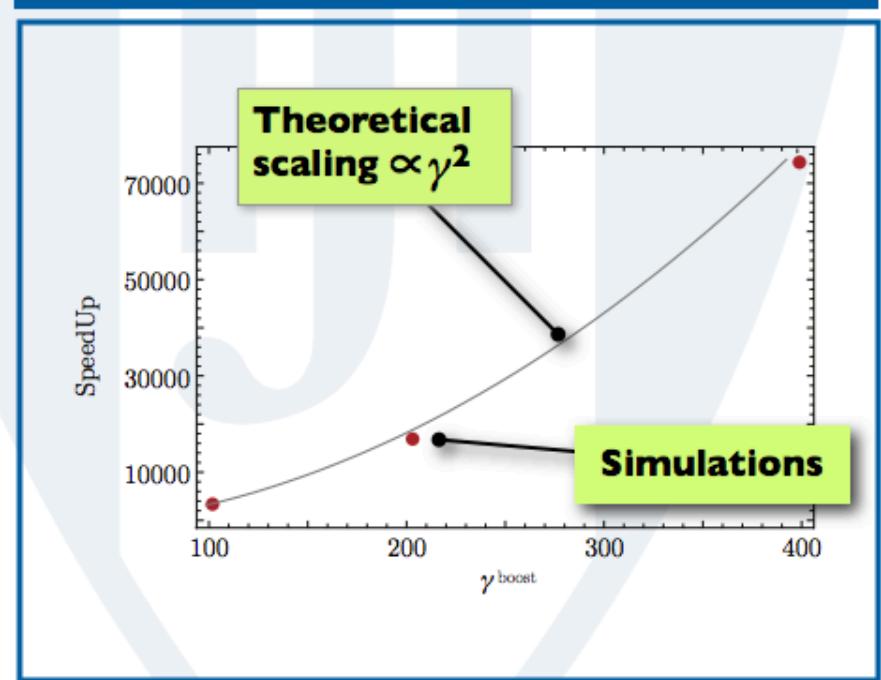
-- Planar antenna enabled high γ boost and high speedups



Simulations with $\gamma^{\text{boost}} \sim 400$



Computational speed ups



See also talk from P. Yu (WG2)

*J.-L. Vay, et al., *Phys. Plasmas* **18** 123103 (2011)

Conclusion

- Particle-In-Cell methodology for the modeling of advanced accelerators is a **very active area of research**.
- Challenges such as space and time scale disparities, discretization errors, numerical dispersion, have pushed toward the **development of better methods**:
 - Fourier multimode solver,
 - improved laser envelope solvers,
 - improved quasistatic solvers,
 - Beam Frame Poisson Solver,
 - Lorentz invariant particle pusher,
 - Lorentz boosted frame,
 - PIC w/ tunable electromagnetic field solver,
 - strided filtering,
 - laser injection through moving plane.
- The novel algorithms are quite general and have **broad applicability**.
- Much to explore with **exciting possibilities**:
 - combination of techniques (e.g. Fourier multimode solver + boosted frame)
 - node based electromagnetic solvers (high order, Fourier, etc)
 - GPU/manycores,
 - mesh refinement,
 - ...